



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:58 AM UTC

PDB ID : 5UW6 / pdb_00005uw6
Title : PCY1 in Complex with Follower Peptide and Covalent Inhibitor ZPP
Authors : Chekan, J.R.; Nair, S.K.
Deposited on : 2017-02-20
Resolution : 3.30 Å(reported)

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

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

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

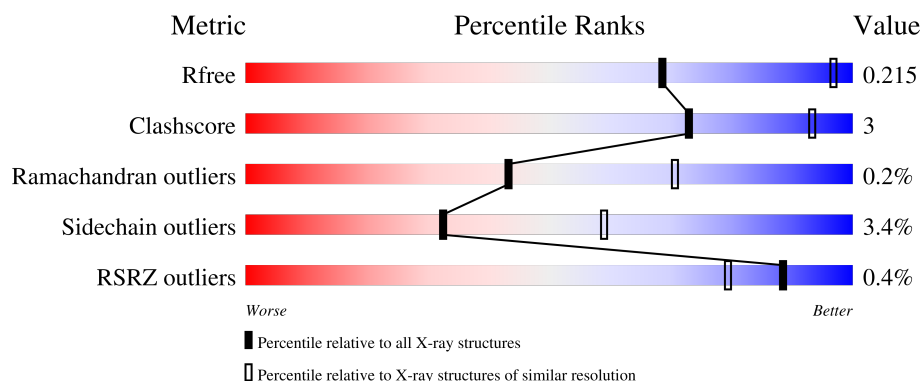
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	750	% 83% 9% • 8%
1	B	750	85% 9% • 6%
1	C	750	% 85% 8% •• 7%
1	D	750	85% 7% • 7%
2	E	6	100%

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Mol	Chain	Length	Quality of chain
2	F	6	 100%
2	G	6	 83% 17%
2	H	6	 83% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22866 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptide cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	7	0
			5633	3600	957	1050	26			
1	B	706	Total	C	N	O	S	0	0	0
			5661	3617	962	1057	25			
1	C	701	Total	C	N	O	S	0	3	0
			5665	3623	966	1050	26			
1	D	697	Total	C	N	O	S	0	0	0
			5601	3582	953	1041	25			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP R4P353
A	-24	SER	-	expression tag	UNP R4P353
A	-23	TYR	-	expression tag	UNP R4P353
A	-22	TYR	-	expression tag	UNP R4P353
A	-21	HIS	-	expression tag	UNP R4P353
A	-20	HIS	-	expression tag	UNP R4P353
A	-19	HIS	-	expression tag	UNP R4P353
A	-18	HIS	-	expression tag	UNP R4P353
A	-17	HIS	-	expression tag	UNP R4P353
A	-16	HIS	-	expression tag	UNP R4P353
A	-15	LEU	-	expression tag	UNP R4P353
A	-14	GLU	-	expression tag	UNP R4P353
A	-13	SER	-	expression tag	UNP R4P353
A	-12	THR	-	expression tag	UNP R4P353
A	-11	SER	-	expression tag	UNP R4P353
A	-10	LEU	-	expression tag	UNP R4P353
A	-9	TYR	-	expression tag	UNP R4P353
A	-8	LYS	-	expression tag	UNP R4P353
A	-7	LYS	-	expression tag	UNP R4P353
A	-6	ALA	-	expression tag	UNP R4P353
A	-5	GLY	-	expression tag	UNP R4P353

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP R4P353
A	-3	GLU	-	expression tag	UNP R4P353
A	-2	PHE	-	expression tag	UNP R4P353
A	-1	ALA	-	expression tag	UNP R4P353
A	0	LEU	-	expression tag	UNP R4P353
B	-25	MET	-	initiating methionine	UNP R4P353
B	-24	SER	-	expression tag	UNP R4P353
B	-23	TYR	-	expression tag	UNP R4P353
B	-22	TYR	-	expression tag	UNP R4P353
B	-21	HIS	-	expression tag	UNP R4P353
B	-20	HIS	-	expression tag	UNP R4P353
B	-19	HIS	-	expression tag	UNP R4P353
B	-18	HIS	-	expression tag	UNP R4P353
B	-17	HIS	-	expression tag	UNP R4P353
B	-16	HIS	-	expression tag	UNP R4P353
B	-15	LEU	-	expression tag	UNP R4P353
B	-14	GLU	-	expression tag	UNP R4P353
B	-13	SER	-	expression tag	UNP R4P353
B	-12	THR	-	expression tag	UNP R4P353
B	-11	SER	-	expression tag	UNP R4P353
B	-10	LEU	-	expression tag	UNP R4P353
B	-9	TYR	-	expression tag	UNP R4P353
B	-8	LYS	-	expression tag	UNP R4P353
B	-7	LYS	-	expression tag	UNP R4P353
B	-6	ALA	-	expression tag	UNP R4P353
B	-5	GLY	-	expression tag	UNP R4P353
B	-4	SER	-	expression tag	UNP R4P353
B	-3	GLU	-	expression tag	UNP R4P353
B	-2	PHE	-	expression tag	UNP R4P353
B	-1	ALA	-	expression tag	UNP R4P353
B	0	LEU	-	expression tag	UNP R4P353
C	-25	MET	-	initiating methionine	UNP R4P353
C	-24	SER	-	expression tag	UNP R4P353
C	-23	TYR	-	expression tag	UNP R4P353
C	-22	TYR	-	expression tag	UNP R4P353
C	-21	HIS	-	expression tag	UNP R4P353
C	-20	HIS	-	expression tag	UNP R4P353
C	-19	HIS	-	expression tag	UNP R4P353
C	-18	HIS	-	expression tag	UNP R4P353
C	-17	HIS	-	expression tag	UNP R4P353
C	-16	HIS	-	expression tag	UNP R4P353
C	-15	LEU	-	expression tag	UNP R4P353

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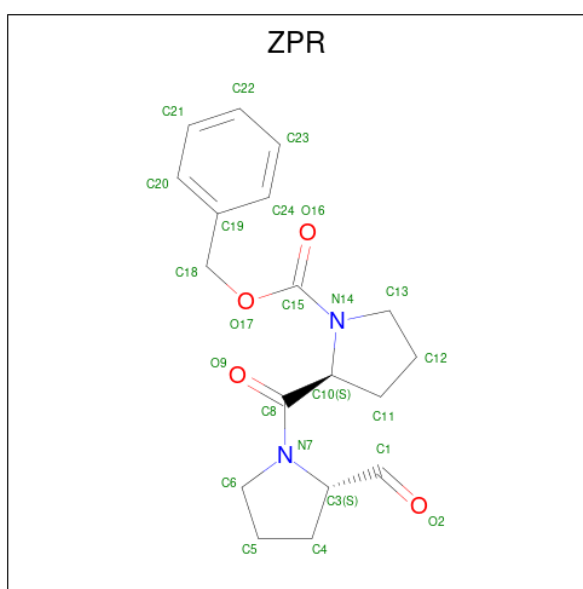
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	GLU	-	expression tag	UNP R4P353
C	-13	SER	-	expression tag	UNP R4P353
C	-12	THR	-	expression tag	UNP R4P353
C	-11	SER	-	expression tag	UNP R4P353
C	-10	LEU	-	expression tag	UNP R4P353
C	-9	TYR	-	expression tag	UNP R4P353
C	-8	LYS	-	expression tag	UNP R4P353
C	-7	LYS	-	expression tag	UNP R4P353
C	-6	ALA	-	expression tag	UNP R4P353
C	-5	GLY	-	expression tag	UNP R4P353
C	-4	SER	-	expression tag	UNP R4P353
C	-3	GLU	-	expression tag	UNP R4P353
C	-2	PHE	-	expression tag	UNP R4P353
C	-1	ALA	-	expression tag	UNP R4P353
C	0	LEU	-	expression tag	UNP R4P353
D	-25	MET	-	initiating methionine	UNP R4P353
D	-24	SER	-	expression tag	UNP R4P353
D	-23	TYR	-	expression tag	UNP R4P353
D	-22	TYR	-	expression tag	UNP R4P353
D	-21	HIS	-	expression tag	UNP R4P353
D	-20	HIS	-	expression tag	UNP R4P353
D	-19	HIS	-	expression tag	UNP R4P353
D	-18	HIS	-	expression tag	UNP R4P353
D	-17	HIS	-	expression tag	UNP R4P353
D	-16	HIS	-	expression tag	UNP R4P353
D	-15	LEU	-	expression tag	UNP R4P353
D	-14	GLU	-	expression tag	UNP R4P353
D	-13	SER	-	expression tag	UNP R4P353
D	-12	THR	-	expression tag	UNP R4P353
D	-11	SER	-	expression tag	UNP R4P353
D	-10	LEU	-	expression tag	UNP R4P353
D	-9	TYR	-	expression tag	UNP R4P353
D	-8	LYS	-	expression tag	UNP R4P353
D	-7	LYS	-	expression tag	UNP R4P353
D	-6	ALA	-	expression tag	UNP R4P353
D	-5	GLY	-	expression tag	UNP R4P353
D	-4	SER	-	expression tag	UNP R4P353
D	-3	GLU	-	expression tag	UNP R4P353
D	-2	PHE	-	expression tag	UNP R4P353
D	-1	ALA	-	expression tag	UNP R4P353
D	0	LEU	-	expression tag	UNP R4P353

- Molecule 2 is a protein called Presegetalin A1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			38	23	7	8			
2	F	6	Total	C	N	O	0	0	0
			39	23	7	9			
2	G	6	Total	C	N	O	0	0	0
			38	23	7	8			
2	H	6	Total	C	N	O	0	0	0
			39	23	7	9			

- Molecule 3 is N-BENZYLOXYCARBONYL-L-PROLYL-L-PROLINAL (CCD ID: ZPR) (formula: $C_{18}H_{22}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	18	2	4		
3	B	1	Total	C	N	O	0	0
			24	18	2	4		
3	C	1	Total	C	N	O	0	0
			24	18	2	4		
3	D	1	Total	C	N	O	0	0
			24	18	2	4		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Ca 2	0	0
4	C	1	Total 1	Ca 1	0	0

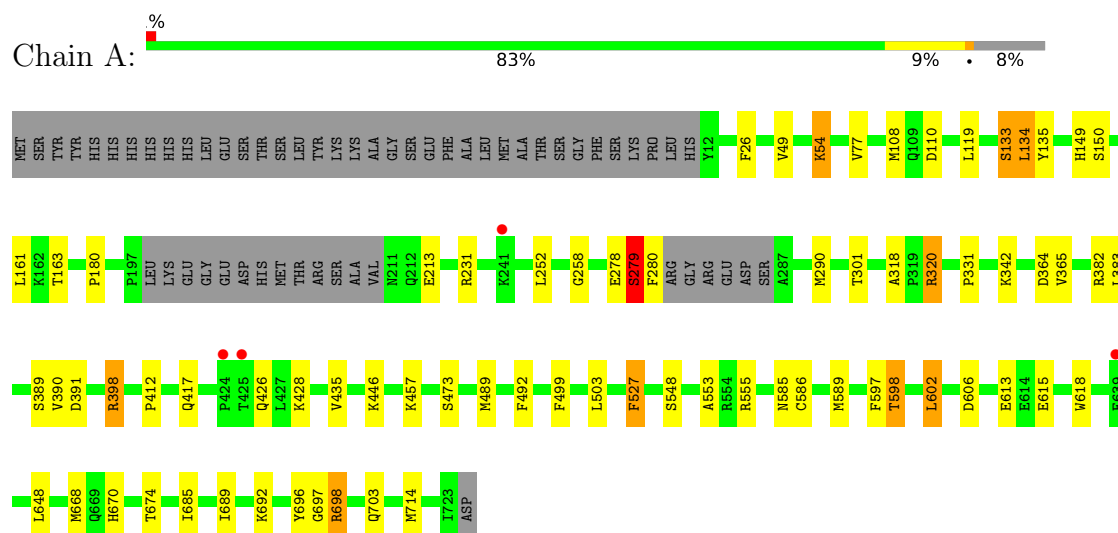
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total 13	O 13	0	0
5	B	16	Total 16	O 16	0	0
5	C	8	Total 8	O 8	0	0
5	D	15	Total 15	O 15	0	0

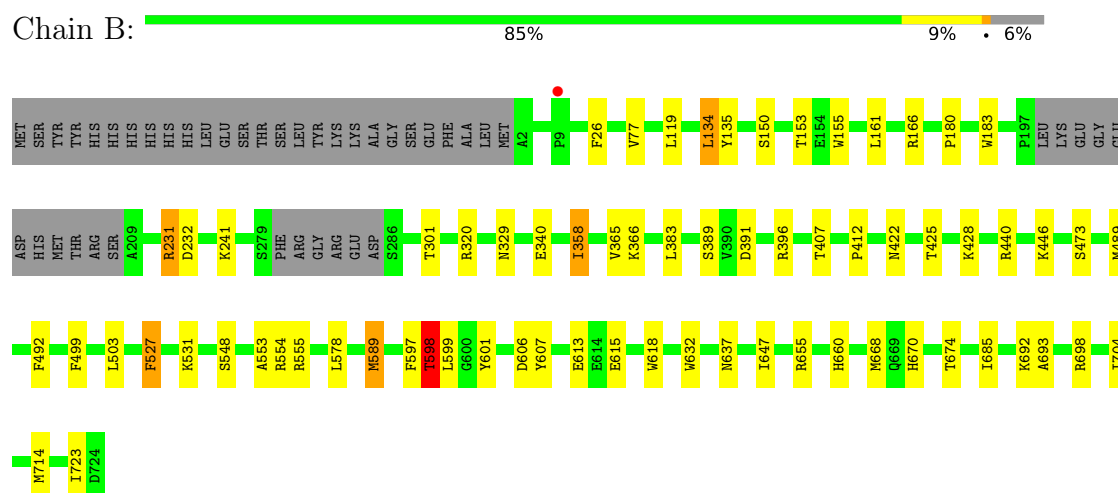
3 Residue-property plots

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.

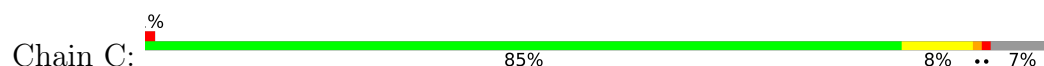
• Molecule 1: Peptide cyclase 1

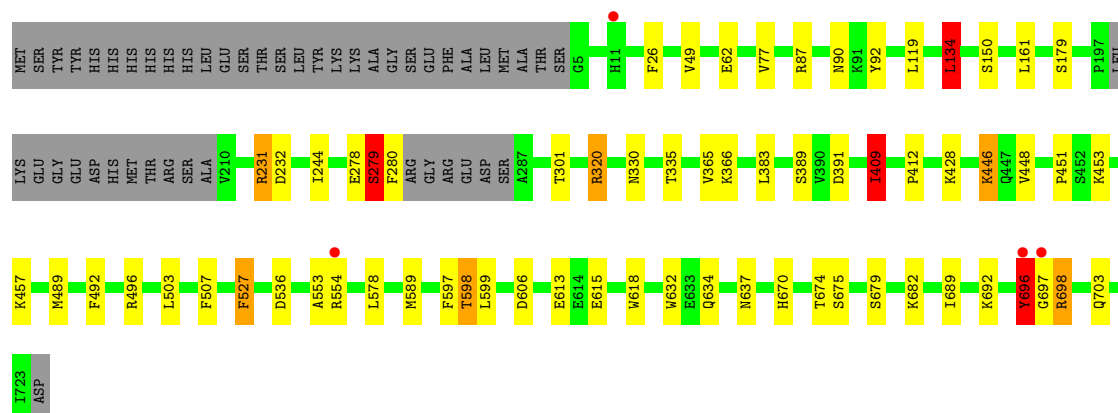


• Molecule 1: Peptide cyclase 1



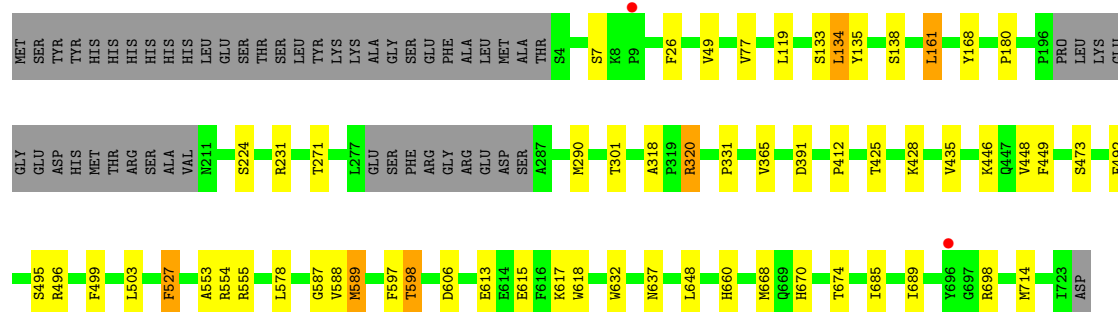
• Molecule 1: Peptide cyclase 1





- Molecule 1: Peptide cyclase 1

Chain D: 85% 7% 7%



- Molecule 2: Presegetalin A1

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: Presegetalin A1

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: Presegetalin A1

Chain G: 83% 17%



- Molecule 2: Presegetalin A1

Chain H: 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.51Å 85.46Å 138.12Å 87.60° 78.17° 89.38°	Depositor
Resolution (Å)	45.20 – 3.30 45.20 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.20-3.30) 98.9 (45.20-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.172 , 0.220 0.173 , 0.215	Depositor DCC
R_{free} test set	2089 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.049 for h,-k,h-l 0.015 for -h,k,-l 0.009 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22866	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: ZPR, CA

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	0.74	0/5777	0.92	8/7821 (0.1%)
1	B	0.74	0/5807	0.94	10/7866 (0.1%)
1	C	0.76	0/5812	0.94	9/7869 (0.1%)
1	D	0.75	0/5746	0.91	4/7781 (0.1%)
2	E	0.77	0/38	0.82	0/52
2	F	0.85	0/39	0.90	0/52
2	G	0.87	0/38	0.98	0/52
2	H	0.92	0/39	0.84	0/52
All	All	0.75	0/23296	0.93	31/31545 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	320	ARG	N-CA-C	-11.01	95.99	110.53
1	D	320	ARG	N-CA-C	-10.20	96.78	110.55
1	A	320	ARG	N-CA-C	-10.07	96.96	110.55
1	D	589	MET	N-CA-C	-9.61	96.11	109.95
1	B	589	MET	N-CA-C	-9.39	95.12	109.96
1	B	704	ILE	CA-CB-CG1	8.82	125.39	110.40
1	C	589	MET	N-CA-C	8.24	124.01	113.88
1	A	553	ALA	N-CA-C	-7.99	98.64	110.23
1	A	589	MET	N-CA-C	7.90	123.60	113.88
1	B	598	THR	CB-CA-C	-7.87	94.75	110.42
1	C	232	ASP	N-CA-C	7.28	119.43	110.91
1	B	232	ASP	N-CA-C	7.11	119.23	110.91
1	C	134	LEU	CA-CB-CG	6.67	139.63	116.30
1	C	231	ARG	N-CA-C	6.48	124.60	110.80
1	B	358	ILE	CB-CA-C	6.48	120.19	111.19
1	C	279	SER	N-CA-C	-6.37	101.26	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	704	ILE	CB-CA-C	-6.27	103.57	112.22
1	A	435	VAL	CB-CA-C	-6.01	105.35	110.94
1	B	723	ILE	N-CA-C	6.00	116.64	107.77
1	B	231	ARG	N-CA-C	5.83	123.23	110.80
1	C	696	TYR	N-CA-C	5.78	123.10	110.80
1	D	435	VAL	CB-CA-C	-5.51	105.81	110.94
1	C	161	LEU	CB-CA-C	-5.28	100.61	109.48
1	A	398	ARG	CB-CA-C	5.27	119.84	109.72
1	A	390	VAL	CB-CA-C	-5.26	103.36	111.31
1	C	409	ILE	CA-CB-CG1	5.22	119.27	110.40
1	B	161	LEU	CB-CA-C	-5.11	100.89	109.48
1	A	382	ARG	CB-CG-CD	5.11	123.04	111.30
1	A	279	SER	N-CA-C	-5.10	103.20	110.35
1	D	496	ARG	CG-CD-NE	5.08	123.18	112.00
1	B	607	TYR	N-CA-C	5.03	119.44	112.45

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	5633	0	5472	41	0
1	B	5661	0	5502	34	0
1	C	5665	0	5512	38	0
1	D	5601	0	5449	37	0
2	E	38	0	36	0	0
2	F	39	0	36	0	0
2	G	38	0	36	1	0
2	H	39	0	36	1	0
3	A	24	0	21	0	0
3	B	24	0	21	0	0
3	C	24	0	21	0	0
3	D	24	0	21	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
5	A	13	0	0	0	0
5	B	16	0	0	6	0
5	C	8	0	0	2	0
5	D	15	0	0	2	0
All	All	22866	0	22163	142	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 3.

All (142) 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:108:MET:HE1	1:A:163:THR:HB	1.49	0.92
1:C:682:LYS:HG2	5:C:901:HOH:O	1.81	0.79
1:C:446:LYS:HE3	1:C:448:VAL:CG1	2.23	0.67
1:A:342:LYS:HD2	1:C:366:LYS:HE3	1.77	0.67
1:A:698:ARG:HD3	1:A:703:GLN:OE1	1.97	0.65
1:C:446:LYS:HE3	1:C:448:VAL:HG13	1.81	0.62
1:C:446:LYS:CE	1:C:448:VAL:CG1	2.77	0.62
1:A:668:MET:HB3	1:A:685[B]:ILE:HD13	1.83	0.61
1:B:598:THR:O	1:B:598:THR:OG1	2.10	0.61
1:B:320:ARG:O	1:B:340:GLU:HG3	2.02	0.60
1:D:473:SER:O	1:D:555:ARG:NH2	2.35	0.59
1:B:647:ILE:HG23	5:B:907:HOH:O	2.03	0.58
1:D:448:VAL:HG22	1:D:449:PHE:N	2.17	0.58
1:D:224:SER:OG	5:D:901:HOH:O	1.96	0.58
1:A:258:GLY:HA2	1:A:602:LEU:HB2	1.84	0.58
1:C:279:SER:O	1:C:280:PHE:CG	2.57	0.57
1:A:668:MET:CB	1:A:685[B]:ILE:HD13	2.34	0.57
1:D:588:VAL:N	1:D:589:MET:HE2	2.20	0.55
1:A:110:ASP:HB3	1:D:271:THR:HB	1.87	0.55
1:B:134:LEU:HD12	1:B:135:TYR:N	2.21	0.55
1:A:364:ASP:OD2	1:C:457:LYS:HE2	2.06	0.55
1:D:588:VAL:C	1:D:589:MET:HE2	2.32	0.55
1:D:587:GLY:HA3	1:D:589:MET:CE	2.37	0.54
1:D:134:LEU:HD12	1:D:135:TYR:N	2.23	0.54
1:D:134:LEU:HD13	1:D:180:PRO:HA	1.89	0.54
1:A:134:LEU:HD12	1:A:135:TYR:N	2.23	0.53
1:C:696:TYR:CD2	1:C:697:GLY:N	2.76	0.53
1:A:134:LEU:HD13	1:A:180:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:SER:O	5:C:901:HOH:O	2.19	0.52
1:B:134:LEU:HD13	1:B:180:PRO:HA	1.91	0.52
1:D:587:GLY:HA3	1:D:589:MET:HE3	1.90	0.52
1:B:396:ARG:NH2	5:B:901:HOH:O	2.32	0.51
1:D:589:MET:O	1:D:660:HIS:ND1	2.44	0.51
1:A:499:PHE:CE1	1:A:714:MET:HE1	2.46	0.50
1:B:553:ALA:O	1:B:578:LEU:O	2.29	0.50
1:C:446:LYS:CE	1:C:448:VAL:HG12	2.41	0.50
1:D:553:ALA:O	1:D:578:LEU:O	2.30	0.50
1:A:597:PHE:O	1:A:598:THR:C	2.55	0.49
1:B:597:PHE:O	1:B:598:THR:C	2.54	0.49
1:A:278:GLU:O	1:A:279:SER:C	2.55	0.49
1:B:407:THR:CG2	1:B:492:PHE:H	2.25	0.49
1:A:670:HIS:HA	1:A:674:THR:OG1	2.13	0.49
1:C:670:HIS:HA	1:C:674:THR:OG1	2.12	0.49
1:D:670:HIS:HA	1:D:674:THR:OG1	2.12	0.49
1:D:587:GLY:C	1:D:589:MET:CE	2.86	0.49
1:D:499:PHE:CE1	1:D:714:MET:HE1	2.48	0.48
1:A:698:ARG:CD	1:A:703:GLN:OE1	2.61	0.48
1:A:290[B]:MET:HE1	1:A:331:PRO:HG3	1.95	0.48
1:C:446:LYS:HE2	1:C:448:VAL:CG1	2.43	0.48
1:C:553:ALA:O	1:C:578:LEU:O	2.31	0.48
1:C:598:THR:HB	1:C:599:LEU:HD12	1.95	0.48
1:D:597:PHE:O	1:D:598:THR:C	2.57	0.48
1:B:499:PHE:CE1	1:B:714:MET:HE1	2.48	0.48
1:C:698:ARG:H	1:C:698:ARG:HD2	1.78	0.48
1:A:668:MET:HE2	1:A:685[B]:ILE:HD13	1.96	0.48
1:C:597:PHE:O	1:C:598:THR:C	2.56	0.48
1:C:703:GLN:HG3	2:G:32:VAL:HG21	1.96	0.48
1:A:108:MET:SD	1:A:119:LEU:HD13	2.54	0.48
1:B:613:GLU:HB3	1:D:617:LYS:NZ	2.29	0.47
1:A:499:PHE:CD1	1:A:714:MET:HE1	2.49	0.47
1:D:527:PHE:C	1:D:527:PHE:CD1	2.92	0.47
1:C:615:GLU:HG2	1:C:618:TRP:CH2	2.49	0.47
1:D:615:GLU:HG2	1:D:618:TRP:CH2	2.50	0.47
1:A:527:PHE:C	1:A:527:PHE:CD1	2.91	0.47
1:D:26:PHE:CD1	1:D:613:GLU:HB2	2.50	0.47
1:D:499:PHE:CD1	1:D:714:MET:HE1	2.49	0.47
1:B:183:TRP:HB3	5:B:906:HOH:O	2.14	0.47
1:B:366:LYS:HE3	5:B:912:HOH:O	2.15	0.47
1:B:670:HIS:HA	1:B:674:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:PHE:CD1	1:C:613:GLU:HB2	2.50	0.47
1:D:587:GLY:C	1:D:589:MET:HE2	2.39	0.47
1:B:499:PHE:CD1	1:B:714:MET:HE1	2.50	0.47
1:B:589:MET:O	1:B:660:HIS:ND1	2.47	0.46
1:C:446:LYS:HE3	1:C:448:VAL:HG12	1.96	0.46
1:B:599:LEU:HA	1:B:601:TYR:CE1	2.51	0.46
1:C:527:PHE:C	1:C:527:PHE:CD1	2.93	0.46
1:A:279:SER:O	1:A:280:PHE:CG	2.69	0.46
1:A:473:SER:O	1:A:555:ARG:NH1	2.49	0.46
1:B:473:SER:O	1:B:555:ARG:NH1	2.49	0.46
1:C:278:GLU:O	1:C:279:SER:C	2.55	0.45
1:A:26:PHE:CD1	1:A:613:GLU:HB2	2.52	0.45
1:C:87[A]:ARG:HE	1:C:90:ASN:HA	1.81	0.45
1:A:54:LYS:CD	1:A:54:LYS:C	2.89	0.45
1:C:412:PRO:HA	1:C:492:PHE:CG	2.51	0.45
1:A:318:ALA:C	1:A:320:ARG:O	2.60	0.45
1:B:527:PHE:CD1	1:B:527:PHE:C	2.93	0.45
1:C:670:HIS:CD2	1:C:675:SER:HB3	2.52	0.45
1:D:138:SER:HB2	5:D:903:HOH:O	2.17	0.45
1:C:391:ASP:OD1	1:C:391:ASP:C	2.60	0.45
1:A:391:ASP:OD1	1:A:391:ASP:C	2.59	0.44
1:B:26:PHE:CD1	1:B:613:GLU:HB2	2.52	0.44
1:A:279:SER:O	1:A:280:PHE:CB	2.66	0.44
1:A:615:GLU:HG2	1:A:618:TRP:CH2	2.53	0.44
1:B:615:GLU:HG2	1:B:618:TRP:CH2	2.52	0.44
1:B:389:SER:HB2	1:B:489:MET:HB3	2.00	0.44
1:B:391:ASP:OD1	1:B:391:ASP:C	2.60	0.44
1:A:412:PRO:HA	1:A:492:PHE:CG	2.53	0.44
1:B:422:ASN:OD1	1:C:330:ASN:ND2	2.51	0.44
1:A:668:MET:HB2	1:A:685[B]:ILE:CD1	2.49	0.43
1:D:161:LEU:HD11	1:D:168:TYR:CE1	2.54	0.43
1:D:648:LEU:N	1:D:648:LEU:HD12	2.32	0.43
1:B:531:LYS:NZ	5:B:903:HOH:O	2.36	0.42
1:C:134:LEU:HD12	1:C:179:SER:O	2.19	0.42
1:D:412:PRO:HA	1:D:492:PHE:CG	2.53	0.42
1:A:389:SER:HB2	1:A:489:MET:HB3	2.01	0.42
1:C:49:VAL:HG13	1:C:689:ILE:HD13	2.01	0.42
1:D:448:VAL:CG2	1:D:449:PHE:N	2.82	0.42
1:C:632:TRP:HA	1:C:637:ASN:O	2.19	0.42
1:B:440:ARG:HH11	1:B:440:ARG:HG3	1.84	0.42
1:C:87[A]:ARG:HD3	1:C:92:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685[B]:ILE:O	1:A:685[B]:ILE:HG13	2.12	0.42
1:C:409:ILE:HD12	1:C:496:ARG:NH1	2.34	0.42
1:A:457:LYS:HB3	1:C:451:PRO:HD3	2.01	0.42
1:A:585:ASN:O	1:A:586:CYS:C	2.63	0.42
1:D:318:ALA:C	1:D:320:ARG:O	2.62	0.42
1:C:698:ARG:HD3	1:C:703:GLN:OE1	2.20	0.42
1:D:391:ASP:C	1:D:391:ASP:OD1	2.63	0.42
1:A:133:SER:HB2	1:A:149:HIS:HE1	1.85	0.41
1:A:213:GLU:HG2	1:A:231:ARG:HG2	2.02	0.41
1:A:696:TYR:CD1	1:A:696:TYR:C	2.98	0.41
1:B:153:THR:HG23	1:B:155:TRP:H	1.85	0.41
1:B:412:PRO:HA	1:B:492:PHE:CG	2.54	0.41
1:B:632:TRP:HA	1:B:637:ASN:O	2.20	0.41
1:A:49:VAL:HG13	1:A:689:ILE:HD13	2.02	0.41
1:D:668:MET:HE2	1:D:685:ILE:HD13	2.01	0.41
1:D:49:VAL:HG13	1:D:689:ILE:HD13	2.03	0.41
1:B:329:ASN:O	1:D:331:PRO:HD2	2.20	0.41
1:B:693:ALA:HB1	1:B:698:ARG:HD2	2.02	0.41
1:D:632:TRP:HA	1:D:637:ASN:O	2.20	0.41
1:B:366:LYS:HB3	5:B:912:HOH:O	2.20	0.41
1:C:134:LEU:CD1	1:C:179:SER:O	2.69	0.41
1:D:495:SER:OG	2:H:32:VAL:OXT	2.31	0.41
1:A:252:LEU:HD12	1:A:252:LEU:N	2.36	0.41
1:A:668:MET:HE2	1:A:685[A]:ILE:HD13	2.02	0.41
1:B:668:MET:HE2	1:B:685:ILE:HD13	2.02	0.40
1:B:613:GLU:HB3	1:D:617:LYS:HZ2	1.86	0.40
1:C:389:SER:HB2	1:C:489:MET:HB3	2.03	0.40
1:C:453:LYS:HE2	1:C:536:ASP:OD1	2.22	0.40
1:C:496:ARG:HD3	1:C:507:PHE:CD2	2.57	0.40
1:A:648:LEU:HD12	1:A:648:LEU:N	2.36	0.40
1:D:473:SER:O	1:D:555:ARG:CZ	2.69	0.40
1:D:587:GLY:CA	1:D:589:MET:HE3	2.50	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	694/750 (92%)	658 (95%)	34 (5%)	2 (0%)	36	65
1	B	700/750 (93%)	663 (95%)	36 (5%)	1 (0%)	48	75
1	C	698/750 (93%)	662 (95%)	34 (5%)	2 (0%)	36	65
1	D	691/750 (92%)	654 (95%)	36 (5%)	1 (0%)	48	75
2	E	4/6 (67%)	4 (100%)	0	0	100	100
2	F	4/6 (67%)	4 (100%)	0	0	100	100
2	G	4/6 (67%)	4 (100%)	0	0	100	100
2	H	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2799/3024 (93%)	2653 (95%)	140 (5%)	6 (0%)	43	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	THR
1	A	697	GLY
1	B	598	THR
1	C	598	THR
1	C	696	TYR
1	D	598	THR

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	610/652 (94%)	588 (96%)	22 (4%)	31	58
1	B	613/652 (94%)	592 (97%)	21 (3%)	32	59
1	C	613/652 (94%)	589 (96%)	24 (4%)	28	56
1	D	606/652 (93%)	588 (97%)	18 (3%)	36	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	4/4 (100%)	4 (100%)	0	100	100
2	F	4/4 (100%)	4 (100%)	0	100	100
2	G	4/4 (100%)	4 (100%)	0	100	100
2	H	4/4 (100%)	4 (100%)	0	100	100
All	All	2458/2624 (94%)	2373 (96%)	85 (4%)	32	58

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	77	VAL
1	A	133	SER
1	A	134	LEU
1	A	150	SER
1	A	161	LEU
1	A	279	SER
1	A	301	THR
1	A	365	VAL
1	A	383	LEU
1	A	398	ARG
1	A	417	GLN
1	A	426	GLN
1	A	428	LYS
1	A	446	LYS
1	A	503	LEU
1	A	527	PHE
1	A	548	SER
1	A	602	LEU
1	A	606	ASP
1	A	692	LYS
1	A	698	ARG
1	B	77	VAL
1	B	119	LEU
1	B	134	LEU
1	B	150	SER
1	B	166	ARG
1	B	231	ARG
1	B	241	LYS
1	B	301	THR
1	B	358	ILE
1	B	365	VAL

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Mol	Chain	Res	Type
1	B	383	LEU
1	B	425	THR
1	B	428	LYS
1	B	446	LYS
1	B	503	LEU
1	B	527	PHE
1	B	548	SER
1	B	554	ARG
1	B	606	ASP
1	B	655	ARG
1	B	692	LYS
1	C	62	GLU
1	C	77	VAL
1	C	119	LEU
1	C	134	LEU
1	C	150	SER
1	C	231	ARG
1	C	244	ILE
1	C	279	SER
1	C	301	THR
1	C	320	ARG
1	C	335	THR
1	C	365	VAL
1	C	383	LEU
1	C	409	ILE
1	C	428	LYS
1	C	446	LYS
1	C	503	LEU
1	C	527	PHE
1	C	554[A]	ARG
1	C	554[B]	ARG
1	C	606	ASP
1	C	634	GLN
1	C	692	LYS
1	C	698	ARG
1	D	7	SER
1	D	77	VAL
1	D	119	LEU
1	D	133	SER
1	D	134	LEU
1	D	161	LEU
1	D	231	ARG

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Mol	Chain	Res	Type
1	D	290	MET
1	D	301	THR
1	D	365	VAL
1	D	425	THR
1	D	428	LYS
1	D	446	LYS
1	D	503	LEU
1	D	527	PHE
1	D	554	ARG
1	D	606	ASP
1	D	698	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	94	HIS
1	A	109	GLN
1	A	149	HIS
1	A	313	GLN
1	A	353	ASN
1	A	356	GLN
1	A	669	GLN
1	A	670	HIS
1	B	90	ASN
1	B	239	HIS
1	B	313	GLN
1	B	353	ASN
1	B	356	GLN
1	B	417	GLN
1	B	585	ASN
1	B	670	HIS
1	B	695	HIS
1	C	107	GLN
1	C	313	GLN
1	C	330	ASN
1	C	353	ASN
1	C	356	GLN
1	C	381	HIS
1	C	563	ASN
1	C	585	ASN
1	C	695	HIS

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Mol	Chain	Res	Type
1	D	94	HIS
1	D	313	GLN
1	D	353	ASN
1	D	356	GLN
1	D	417	GLN
1	D	585	ASN
1	D	670	HIS
1	D	695	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ZPR	B	801	1	25,26,26	1.61	2 (8%)	31,35,35	1.58	5 (16%)
3	ZPR	D	801	1	25,26,26	1.63	2 (8%)	31,35,35	2.10	5 (16%)
3	ZPR	C	801	1	25,26,26	1.25	1 (4%)	31,35,35	2.37	4 (12%)
3	ZPR	A	801	1	25,26,26	1.25	2 (8%)	31,35,35	2.10	2 (6%)

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	ZPR	B	801	1	-	4/17/39/39	0/3/3/3
3	ZPR	D	801	1	-	2/17/39/39	0/3/3/3
3	ZPR	C	801	1	-	6/17/39/39	0/3/3/3
3	ZPR	A	801	1	-	6/17/39/39	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	ZPR	O17-C15	5.98	1.46	1.34
3	B	801	ZPR	O17-C15	5.92	1.46	1.34
3	C	801	ZPR	O17-C15	5.51	1.45	1.34
3	A	801	ZPR	O17-C15	4.76	1.44	1.34
3	D	801	ZPR	C3-N7	-4.50	1.44	1.48
3	B	801	ZPR	C3-N7	-3.60	1.44	1.48
3	A	801	ZPR	C3-N7	-2.21	1.46	1.48

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ZPR	O17-C15-N14	8.79	121.19	111.02
3	D	801	ZPR	O17-C15-N14	8.78	121.18	111.02
3	C	801	ZPR	O17-C15-N14	8.78	121.18	111.02
3	A	801	ZPR	O17-C15-O16	-6.00	114.33	124.76
3	C	801	ZPR	O17-C15-O16	-5.93	114.45	124.76
3	C	801	ZPR	C4-C3-C1	-5.89	104.58	112.66
3	B	801	ZPR	O17-C15-N14	5.09	116.92	111.02
3	D	801	ZPR	O17-C15-O16	-4.62	116.71	124.76
3	B	801	ZPR	C18-O17-C15	3.55	124.45	115.51
3	B	801	ZPR	O17-C15-O16	-3.00	119.55	124.76
3	D	801	ZPR	C4-C3-C1	-2.43	109.32	112.66
3	D	801	ZPR	C13-N14-C15	2.31	128.60	122.94
3	B	801	ZPR	O17-C18-C19	2.26	114.88	109.40
3	B	801	ZPR	C8-C10-N14	2.10	115.75	110.83
3	C	801	ZPR	C8-C10-N14	2.04	115.59	110.83
3	D	801	ZPR	O17-C18-C19	2.03	114.33	109.40

There are no chirality outliers.

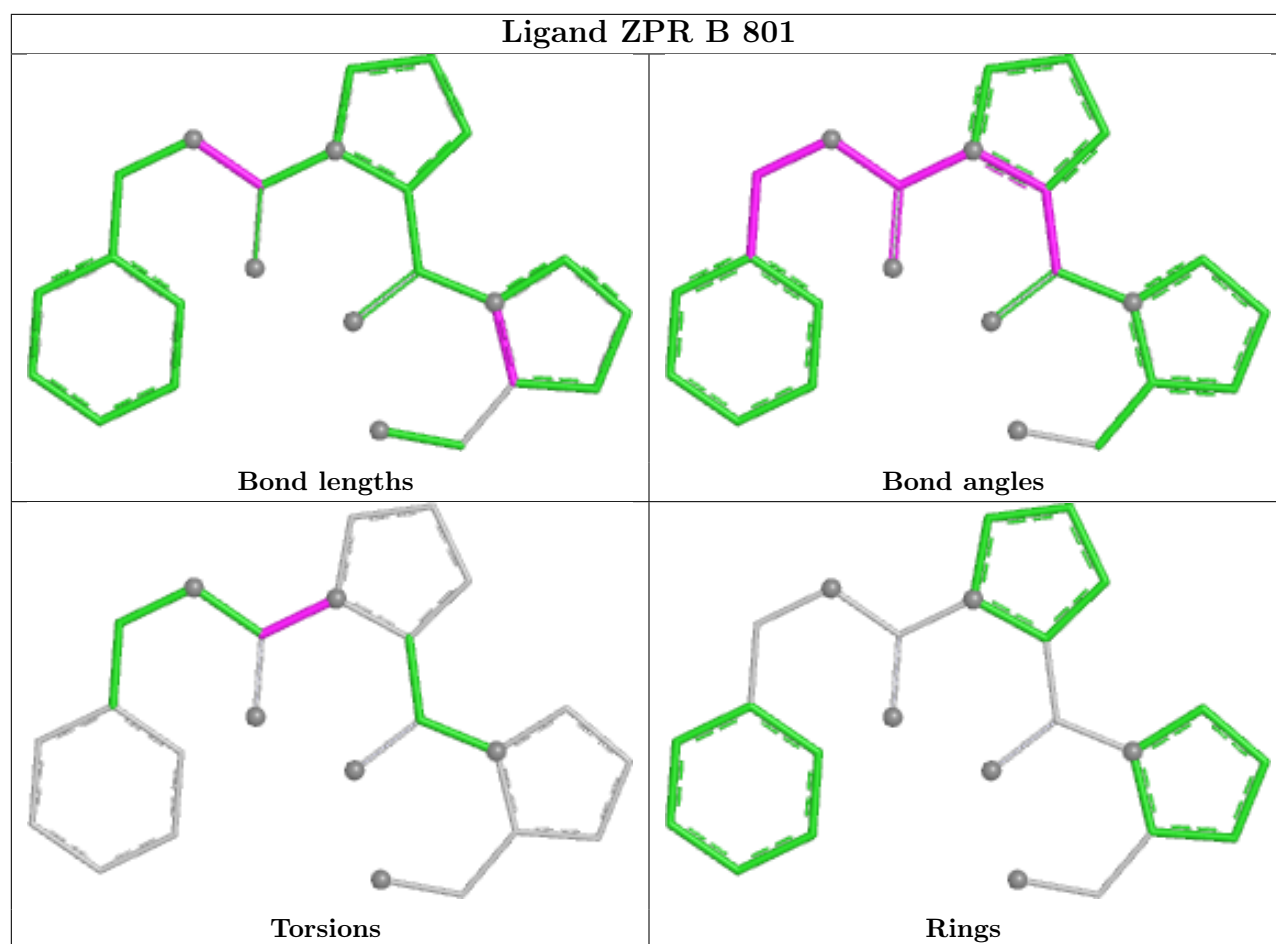
All (18) torsion outliers are listed below:

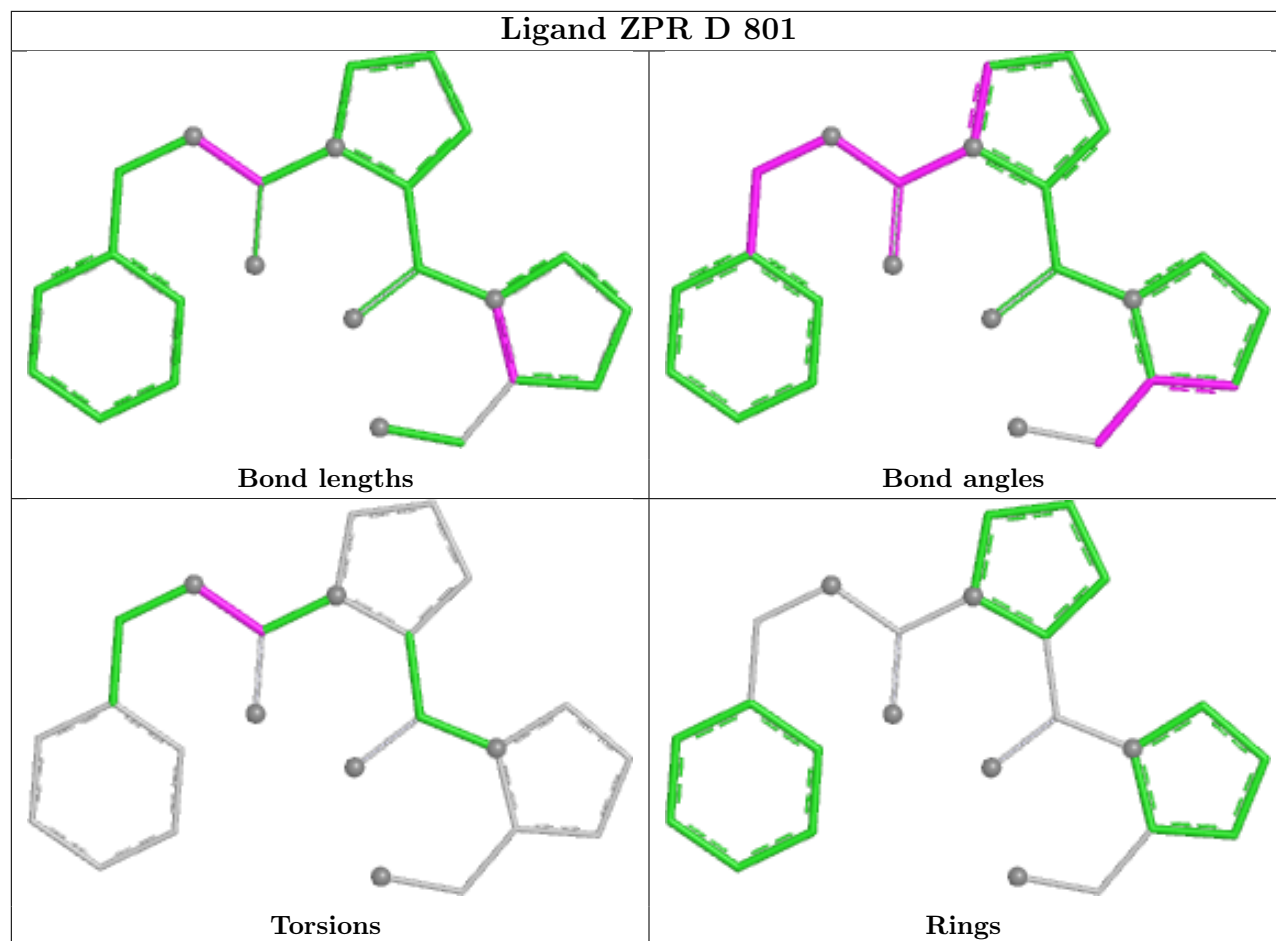
Mol	Chain	Res	Type	Atoms
3	A	801	ZPR	N14-C15-O17-C18
3	A	801	ZPR	O17-C15-N14-C10
3	A	801	ZPR	O17-C15-N14-C13
3	A	801	ZPR	O16-C15-N14-C10
3	A	801	ZPR	O16-C15-N14-C13
3	C	801	ZPR	O16-C15-O17-C18
3	C	801	ZPR	N14-C15-O17-C18
3	C	801	ZPR	O17-C15-N14-C10
3	C	801	ZPR	O17-C15-N14-C13
3	C	801	ZPR	O16-C15-N14-C10
3	C	801	ZPR	O16-C15-N14-C13
3	D	801	ZPR	O16-C15-O17-C18
3	D	801	ZPR	N14-C15-O17-C18
3	A	801	ZPR	O16-C15-O17-C18
3	B	801	ZPR	O17-C15-N14-C10
3	B	801	ZPR	O16-C15-N14-C10
3	B	801	ZPR	O16-C15-N14-C13
3	B	801	ZPR	O17-C15-N14-C13

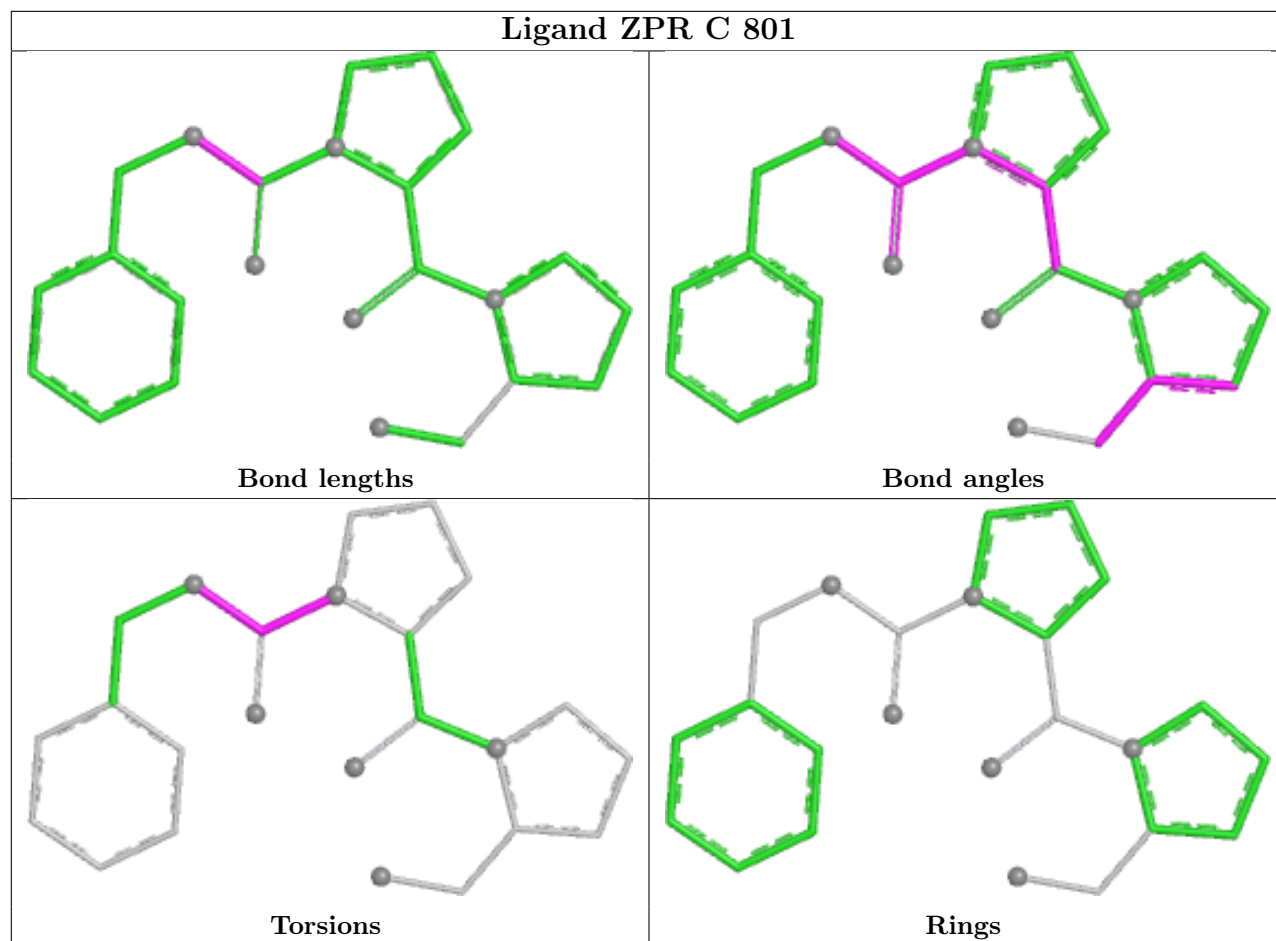
There are no ring outliers.

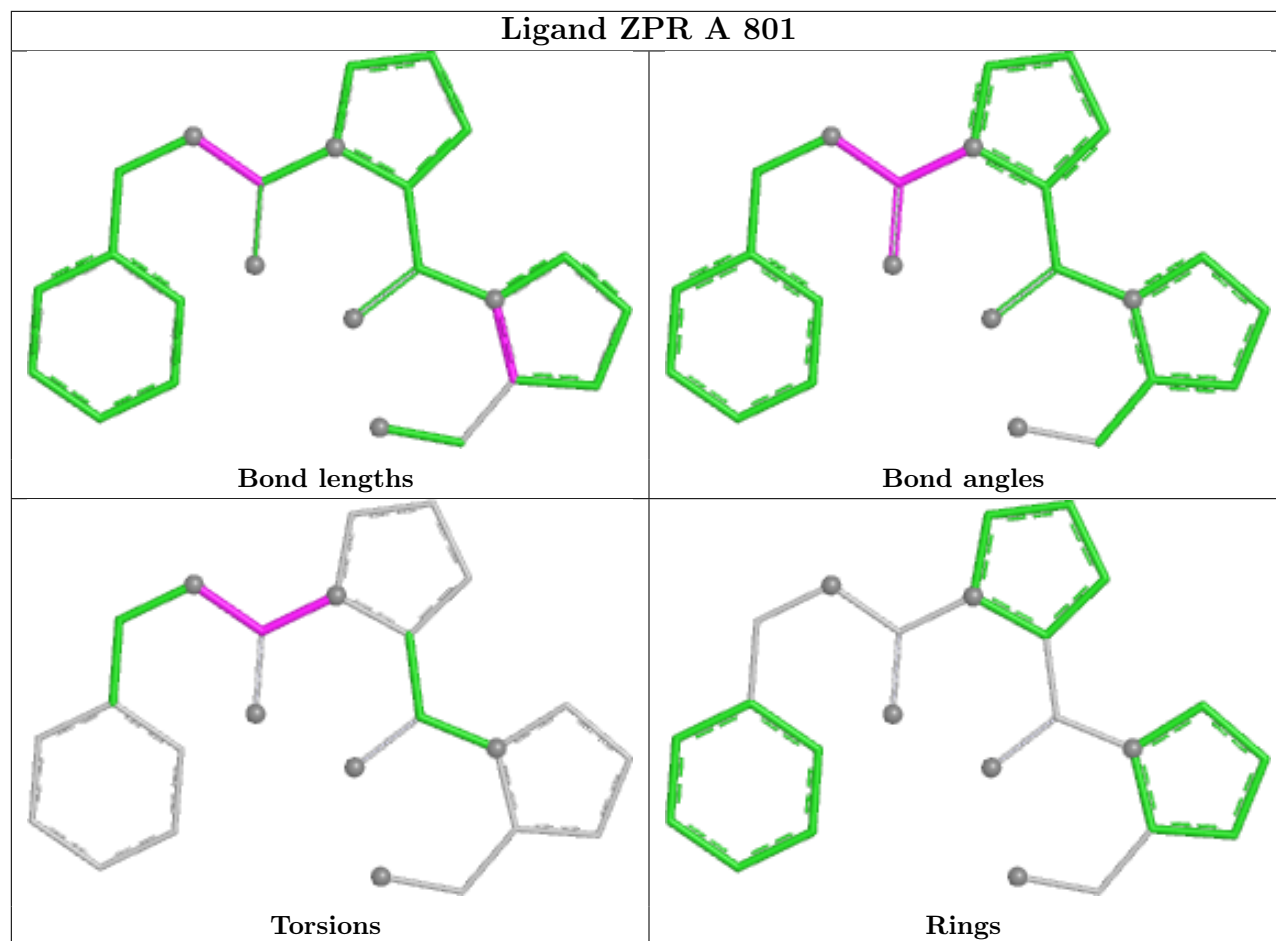
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	693/750 (92%)	-0.29	4 (0%) 85 73	13, 32, 59, 97	7 (1%)
1	B	706/750 (94%)	-0.33	1 (0%) 92 90	17, 30, 58, 92	0
1	C	701/750 (93%)	-0.35	4 (0%) 85 73	10, 28, 56, 97	3 (0%)
1	D	697/750 (92%)	-0.34	2 (0%) 90 82	15, 30, 57, 91	0
2	E	6/6 (100%)	-0.16	0 100 100	33, 41, 52, 56	0
2	F	6/6 (100%)	0.06	0 100 100	27, 36, 53, 55	0
2	G	6/6 (100%)	0.17	0 100 100	30, 36, 56, 57	0
2	H	6/6 (100%)	-0.01	0 100 100	28, 32, 51, 62	0
All	All	2821/3024 (93%)	-0.33	11 (0%) 88 79	10, 30, 58, 97	10 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	THR	3.0
1	C	697	GLY	2.9
1	A	639[A]	GLU	2.9
1	A	424	PRO	2.5
1	D	9	PRO	2.3
1	A	241[A]	LYS	2.2
1	C	11	HIS	2.1
1	D	696	TYR	2.1
1	C	696	TYR	2.1
1	B	9	PRO	2.1
1	C	554[A]	ARG	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](#)

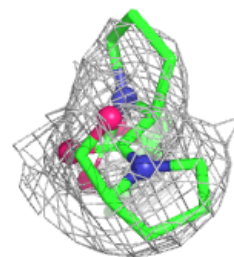
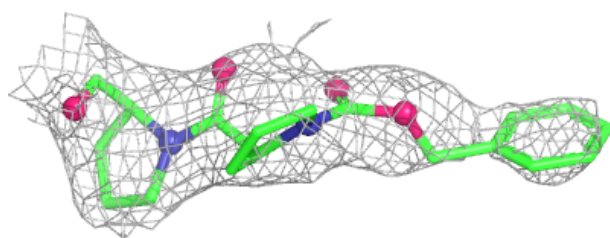
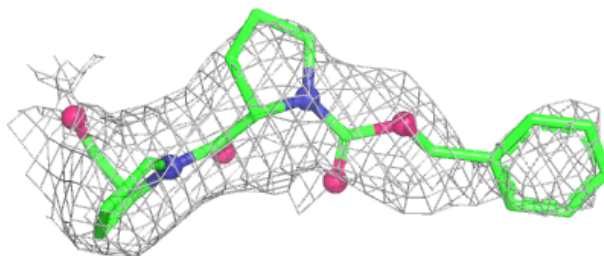
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	ZPR	A	801	24/24	0.93	0.12	41,54,58,62	0
4	CA	B	802	1/1	0.93	0.05	37,37,37,37	0
4	CA	B	803	1/1	0.94	0.05	30,30,30,30	0
3	ZPR	B	801	24/24	0.95	0.11	26,31,56,58	0
3	ZPR	C	801	24/24	0.95	0.09	31,37,48,48	0
4	CA	A	802	1/1	0.96	0.05	41,41,41,41	0
3	ZPR	D	801	24/24	0.97	0.08	33,40,52,53	0
4	CA	C	802	1/1	0.97	0.02	27,27,27,27	0

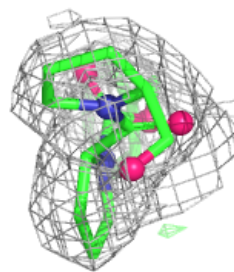
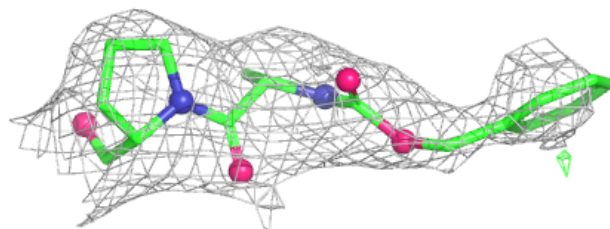
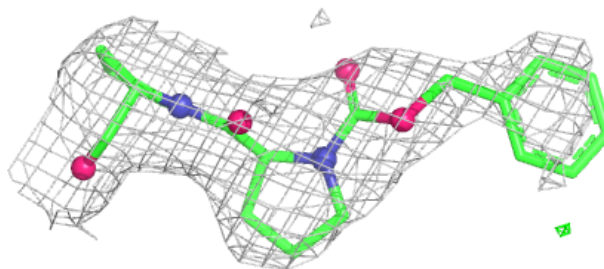
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZPR 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)

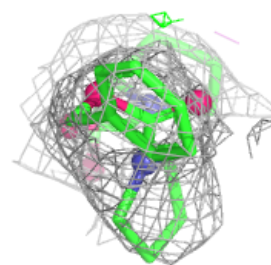
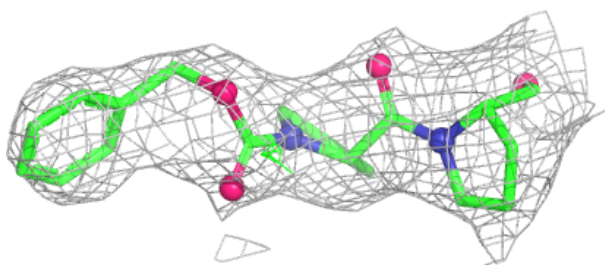
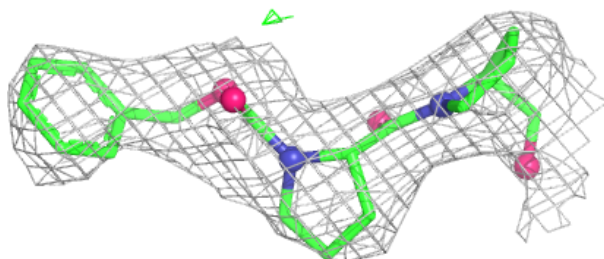
**Electron density around ZPR B 801:**

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

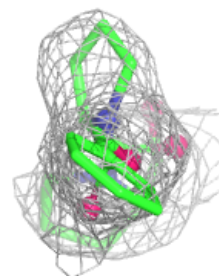
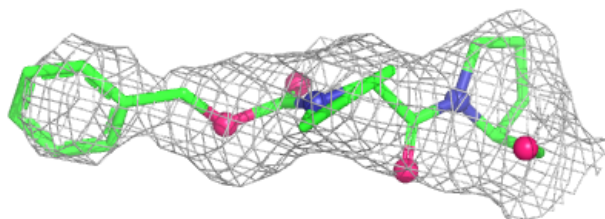
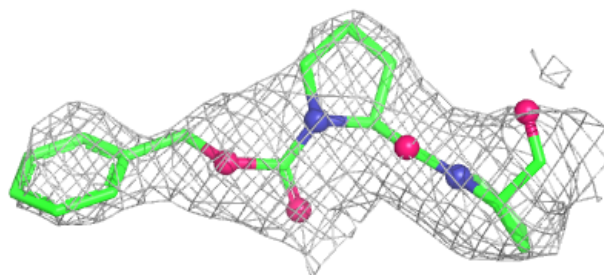


Electron density around ZPR C 801:

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

**Electron density around ZPR D 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.