



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:35 AM UTC

PDB ID : 6GBX / pdb_00006gbx
Title : Crystal structure of human glutaminyl cyclase variant Y115E-Y117E in complex with SEN177
Authors : Pozzi, C.; Di Pisa, F.; Benvenuti, M.; Mangani, S.
Deposited on : 2018-04-16
Resolution : 1.72 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

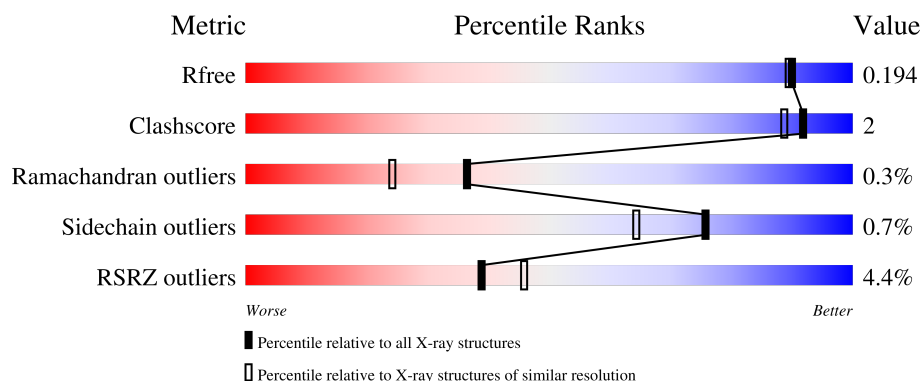
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	329	5% 95% 5%
1	B	329	4% 94% 5%
1	C	329	4% 95% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8792 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	2	0
			2624	1678	453	484	9			
1	B	328	Total	C	N	O	S	0	7	0
			2671	1705	461	496	9			
1	C	328	Total	C	N	O	S	0	3	0
			2627	1679	450	489	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	GLU	TYR	engineered mutation	UNP Q16769
A	117	GLU	TYR	engineered mutation	UNP Q16769
B	115	GLU	TYR	engineered mutation	UNP Q16769
B	117	GLU	TYR	engineered mutation	UNP Q16769
C	115	GLU	TYR	engineered mutation	UNP Q16769
C	117	GLU	TYR	engineered mutation	UNP Q16769

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

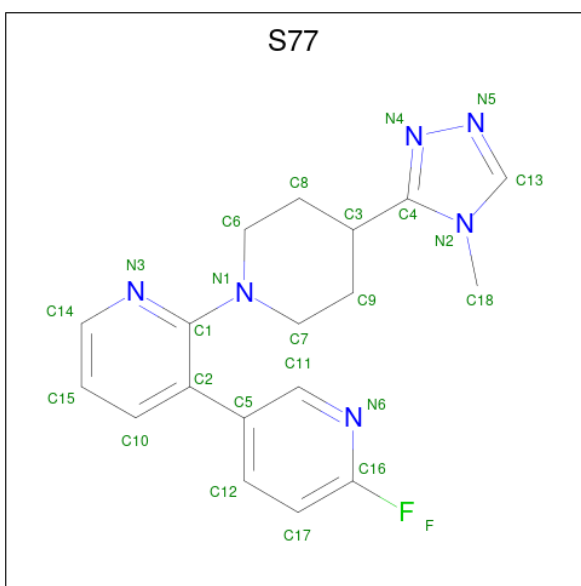
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



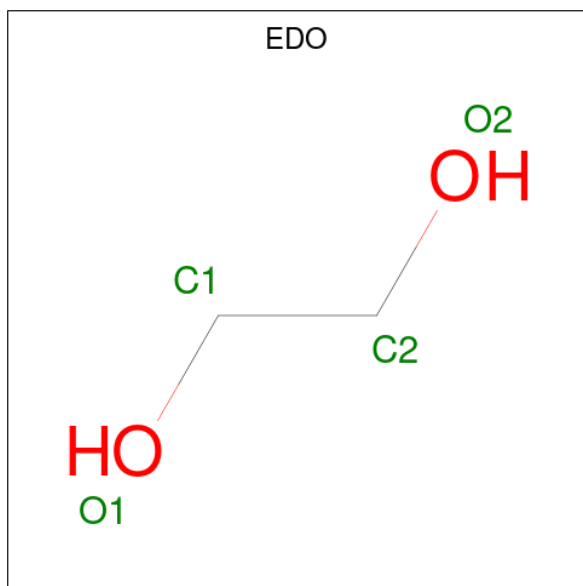
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-fluoranyl-5-[2-[4-(4-methyl-1,2,4-triazol-3-yl)piperidin-1-yl]pyridin-3-yl]pyridine (CCD ID: S77) (formula: C₁₈H₁₉FN₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			25	18	1	6		
4	B	1	Total	C	F	N	0	0
			25	18	1	6		
4	C	1	Total	C	F	N	0	0
			25	18	1	6		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

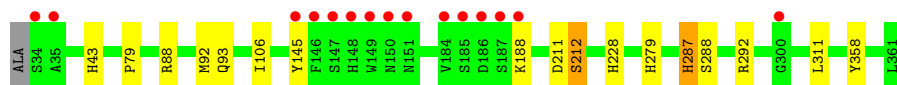
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	235	Total O 235 235	0	0
6	B	233	Total O 233 233	0	0
6	C	229	Total O 229 229	0	0

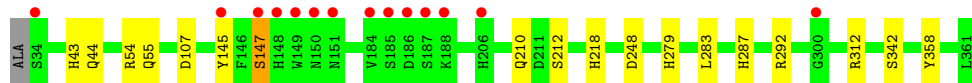
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

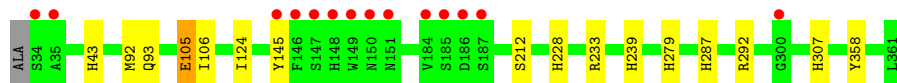
- Molecule 1: Glutaminyl-peptidase cyclotransferase



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- Molecule 1: Glutaminyl-peptidase cyclotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.14Å 149.81Å 95.98Å 90.00° 97.18° 90.00°	Depositor
Resolution (Å)	95.23 – 1.72 95.23 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.23-1.72) 99.8 (95.23-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.158 , 0.183 0.169 , 0.194	Depositor DCC
R_{free} test set	6549 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8792	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: SO4, EDO, S77, ZN

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	0.98	2/2703 (0.1%)	1.00	2/3679 (0.1%)
1	B	0.96	2/2761 (0.1%)	0.97	1/3756 (0.0%)
1	C	1.02	3/2709 (0.1%)	1.00	1/3689 (0.0%)
All	All	0.99	7/8173 (0.1%)	0.99	4/11124 (0.0%)

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	1
1	B	0	2
1	C	0	2
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	239	HIS	CE1-NE2	6.73	1.39	1.32
1	B	342	SER	C-O	-5.50	1.17	1.24
1	B	147	SER	N-CA	5.30	1.52	1.45
1	C	228	HIS	CE1-NE2	5.28	1.37	1.32
1	A	287	HIS	CE1-NE2	5.26	1.37	1.32
1	A	228	HIS	CE1-NE2	5.18	1.37	1.32
1	C	307	HIS	CE1-NE2	5.15	1.37	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	LYS	CB-CA-C	5.96	118.14	109.20
1	A	88	ARG	CB-CA-C	5.34	119.26	110.88
1	B	248	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	105	GLU	CB-CA-C	5.06	119.65	109.38

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	ARG	Sidechain
1	B	292	ARG	Sidechain
1	B	312	ARG	Sidechain
1	C	233	ARG	Sidechain
1	C	292	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2624	0	2547	9	0
1	B	2671	0	2584	10	0
1	C	2627	0	2539	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
4	C	25	0	0	0	0
5	A	20	0	30	0	0
5	B	36	0	54	2	0
5	C	24	0	36	1	0
6	A	235	0	0	1	0
6	B	233	0	0	2	0
6	C	229	0	0	1	0
All	All	8792	0	7790	26	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 2.

All (26) 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:43:HIS:HD2	6:C:659:HOH:O	1.76	0.69
1:B:43:HIS:HD2	6:B:680:HOH:O	1.84	0.60
1:A:279:HIS:HD2	1:A:287:HIS:ND1	2.00	0.60
1:B:279:HIS:HD2	1:B:287:HIS:ND1	2.01	0.59
1:C:43:HIS:HE1	1:C:358:TYR:O	1.85	0.58
1:A:43:HIS:HE1	1:A:358:TYR:O	1.87	0.57
1:A:43:HIS:HD2	6:A:676:HOH:O	1.88	0.56
1:C:279:HIS:HD2	1:C:287:HIS:ND1	2.04	0.56
1:B:145:TYR:CD1	1:B:145:TYR:C	2.85	0.54
1:B:43:HIS:HE1	1:B:358:TYR:O	1.90	0.54
1:B:54[B]:ARG:HD2	1:B:283:LEU:HD21	1.90	0.52
1:A:145:TYR:C	1:A:145:TYR:CD1	2.89	0.51
1:C:145:TYR:CD1	1:C:145:TYR:C	2.89	0.50
1:B:55[A]:GLN:OE1	5:B:412:EDO:O1	2.32	0.48
1:B:279:HIS:CD2	1:B:287:HIS:ND1	2.81	0.48
1:B:44:GLN:NE2	5:B:408:EDO:O1	2.47	0.47
1:A:211:ASP:O	1:A:212:SER:HB3	2.15	0.46
1:B:210[B]:GLN:NE2	6:B:509:HOH:O	2.48	0.46
1:A:279:HIS:CD2	1:A:287:HIS:ND1	2.83	0.46
1:C:279:HIS:CD2	1:C:287:HIS:ND1	2.83	0.45
1:A:92:MET:HE1	1:A:106:ILE:HD11	1.99	0.45
1:C:124:ILE:HD13	5:C:409:EDO:H22	1.99	0.45
1:B:107:ASP:OD1	1:B:218:HIS:HE1	2.01	0.45
1:A:43:HIS:CE1	1:A:358:TYR:O	2.71	0.42
1:A:311:LEU:C	1:A:311:LEU:HD23	2.47	0.40
1:C:92:MET:SD	1:C:106:ILE:HD11	2.61	0.40

There are no symmetry-related clashes.

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	328/329 (100%)	315 (96%)	12 (4%)	1 (0%)	36	24
1	B	333/329 (101%)	323 (97%)	9 (3%)	1 (0%)	36	24
1	C	329/329 (100%)	318 (97%)	10 (3%)	1 (0%)	36	24
All	All	990/987 (100%)	956 (97%)	31 (3%)	3 (0%)	36	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	SER
1	C	212	SER
1	B	212	SER

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	285/290 (98%)	282 (99%)	3 (1%)	65	50
1	B	292/290 (101%)	291 (100%)	1 (0%)	86	79
1	C	286/290 (99%)	284 (99%)	2 (1%)	76	64
All	All	863/870 (99%)	857 (99%)	6 (1%)	76	64

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

Mol	Chain	Res	Type
1	A	79	PRO
1	A	93	GLN
1	A	288	SER
1	B	147	SER
1	C	93	GLN
1	C	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	93	GLN
1	A	218	HIS
1	A	272	GLN
1	A	276	HIS
1	A	279	HIS
1	A	296	ASN
1	A	338	ASN
1	B	43	HIS
1	B	44	GLN
1	B	67	GLN
1	B	99	GLN
1	B	272	GLN
1	B	276	HIS
1	B	279	HIS
1	B	296	ASN
1	B	304	GLN
1	B	338	ASN
1	C	41	ASN
1	C	43	HIS
1	C	93	GLN
1	C	218	HIS
1	C	272	GLN
1	C	279	HIS
1	C	296	ASN
1	C	304	GLN
1	C	338	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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	$\# Z > 2$
5	EDO	A	405	-	3,3,3	0.80	0	2,2,2	0.23	0
5	EDO	A	408	-	3,3,3	0.38	0	2,2,2	0.95	0
5	EDO	B	404	-	3,3,3	0.27	0	2,2,2	0.57	0
5	EDO	A	407	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	B	412	-	3,3,3	0.34	0	2,2,2	0.12	0
5	EDO	C	404	-	3,3,3	0.81	0	2,2,2	0.32	0
3	SO4	C	402	-	4,4,4	0.56	0	6,6,6	0.37	0
3	SO4	B	402	-	4,4,4	0.44	0	6,6,6	0.83	0
5	EDO	B	406	-	3,3,3	0.41	0	2,2,2	0.43	0
5	EDO	B	410	-	3,3,3	0.42	0	2,2,2	0.13	0
5	EDO	C	405	-	3,3,3	0.37	0	2,2,2	0.68	0
4	S77	C	403	2	28,28,28	1.96	7 (25%)	37,39,39	3.13	18 (48%)
5	EDO	C	408	-	3,3,3	0.33	0	2,2,2	0.74	0
5	EDO	C	409	-	3,3,3	0.53	0	2,2,2	0.44	0
4	S77	A	403	2	28,28,28	1.96	12 (42%)	37,39,39	3.61	14 (37%)
5	EDO	B	408	-	3,3,3	0.59	0	2,2,2	0.31	0
5	EDO	B	411	-	3,3,3	0.80	0	2,2,2	0.10	0
3	SO4	A	402	-	4,4,4	0.46	0	6,6,6	0.40	0
5	EDO	C	406	-	3,3,3	0.35	0	2,2,2	0.19	0
5	EDO	A	406	-	3,3,3	0.83	0	2,2,2	0.44	0
5	EDO	A	404	-	3,3,3	0.43	0	2,2,2	0.64	0
4	S77	B	403	2	28,28,28	2.44	11 (39%)	37,39,39	3.27	17 (45%)
5	EDO	B	405	-	3,3,3	0.66	0	2,2,2	0.45	0
5	EDO	B	409	-	3,3,3	0.53	0	2,2,2	0.37	0
5	EDO	C	407	-	3,3,3	0.88	0	2,2,2	0.37	0
5	EDO	B	407	-	3,3,3	0.31	0	2,2,2	0.67	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
5	EDO	A	405	-	-	0/1/1/1	-
5	EDO	A	408	-	-	0/1/1/1	-
5	EDO	B	404	-	-	0/1/1/1	-
5	EDO	A	407	-	-	1/1/1/1	-
5	EDO	B	412	-	-	1/1/1/1	-
5	EDO	C	404	-	-	0/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	B	410	-	-	1/1/1/1	-
5	EDO	C	405	-	-	0/1/1/1	-
4	S77	C	403	2	-	2/12/22/22	0/4/4/4
5	EDO	C	408	-	-	1/1/1/1	-
5	EDO	C	409	-	-	1/1/1/1	-
4	S77	A	403	2	-	2/12/22/22	0/4/4/4
5	EDO	B	408	-	-	0/1/1/1	-
5	EDO	B	411	-	-	0/1/1/1	-
5	EDO	C	406	-	-	0/1/1/1	-
5	EDO	A	406	-	-	0/1/1/1	-
5	EDO	A	404	-	-	0/1/1/1	-
4	S77	B	403	2	-	3/12/22/22	0/4/4/4
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	B	409	-	-	1/1/1/1	-
5	EDO	C	407	-	-	0/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	S77	C8-C3	-4.89	1.40	1.53
4	A	403	S77	C2-C5	-4.74	1.40	1.49
4	B	403	S77	C2-C5	-4.68	1.41	1.49
4	C	403	S77	C2-C5	-4.65	1.41	1.49
4	C	403	S77	C17-C16	4.34	1.42	1.37
4	B	403	S77	C14-N3	4.33	1.43	1.34
4	C	403	S77	C14-N3	4.28	1.43	1.34
4	A	403	S77	C11-N6	3.82	1.42	1.34
4	C	403	S77	C11-N6	3.52	1.41	1.34
4	B	403	S77	C6-N1	-3.40	1.40	1.46
4	B	403	S77	C17-C12	3.38	1.44	1.38
4	B	403	S77	C17-C16	3.35	1.41	1.37
4	B	403	S77	C11-C5	3.34	1.45	1.39
4	B	403	S77	C11-N6	3.10	1.40	1.34
4	B	403	S77	C4-N2	-3.03	1.34	1.36
4	C	403	S77	C4-N2	-3.02	1.34	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	S77	C9-C3	-2.95	1.45	1.53
4	A	403	S77	C18-N2	2.89	1.52	1.46
4	A	403	S77	C16-N6	2.69	1.38	1.31
4	A	403	S77	C14-N3	2.57	1.40	1.34
4	A	403	S77	C4-N2	-2.56	1.34	1.36
4	A	403	S77	C4-N4	2.50	1.34	1.32
4	A	403	S77	C17-C16	-2.42	1.35	1.37
4	B	403	S77	C10-C2	2.38	1.43	1.40
4	A	403	S77	C3-C4	2.25	1.53	1.49
4	C	403	S77	C2-C1	-2.20	1.40	1.42
4	C	403	S77	C11-C5	2.15	1.43	1.39
4	A	403	S77	C8-C3	-2.07	1.47	1.53
4	A	403	S77	N5-N4	-2.05	1.35	1.39
4	A	403	S77	C7-N1	-2.02	1.43	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	S77	C11-N6-C16	15.05	120.58	115.78
4	A	403	S77	C17-C16-N6	-9.54	121.85	126.86
4	C	403	S77	C17-C16-N6	-8.88	122.20	126.86
4	B	403	S77	C17-C16-N6	-7.02	123.18	126.86
4	C	403	S77	C18-N2-C4	-6.75	122.54	127.78
4	B	403	S77	C11-N6-C16	6.65	117.90	115.78
4	B	403	S77	C3-C4-N2	6.64	129.11	123.24
4	C	403	S77	C12-C17-C16	6.51	120.67	116.24
4	B	403	S77	N2-C13-N5	-5.93	105.97	111.39
4	A	403	S77	N2-C4-N4	-5.28	108.90	110.99
4	C	403	S77	C11-N6-C16	5.22	117.44	115.78
4	B	403	S77	C12-C17-C16	5.17	119.77	116.24
4	C	403	S77	N2-C4-N4	-5.13	108.95	110.99
4	B	403	S77	N2-C4-N4	-5.11	108.96	110.99
4	C	403	S77	N2-C13-N5	-5.04	106.79	111.39
4	B	403	S77	C6-C8-C3	4.88	118.27	110.54
4	B	403	S77	C11-C5-C2	-4.82	113.14	121.42
4	C	403	S77	C3-C4-N2	4.55	127.25	123.24
4	B	403	S77	C12-C5-C2	4.47	128.31	120.91
4	A	403	S77	F-C16-N6	4.39	121.55	114.93
4	A	403	S77	N2-C13-N5	-4.15	107.60	111.39
4	B	403	S77	C14-N3-C1	3.79	123.63	115.05
4	B	403	S77	C8-C3-C9	3.69	117.77	110.00
4	A	403	S77	C12-C5-C2	-3.63	114.89	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	S77	C11-C5-C2	3.54	127.50	121.42
4	A	403	S77	C5-C11-N6	-3.40	118.87	124.28
4	C	403	S77	C11-C5-C2	-3.33	115.70	121.42
4	B	403	S77	C18-N2-C4	-3.22	125.28	127.78
4	B	403	S77	C9-C3-C4	3.22	115.40	111.29
4	C	403	S77	C14-N3-C1	3.17	122.23	115.05
4	A	403	S77	C14-N3-C1	3.15	122.19	115.05
4	B	403	S77	C15-C14-N3	-3.15	118.44	123.42
4	B	403	S77	C8-C3-C4	3.02	115.15	111.29
4	A	403	S77	C12-C17-C16	3.02	118.30	116.24
4	C	403	S77	C8-C3-C4	-2.99	107.47	111.29
4	C	403	S77	C9-C3-C4	-2.96	107.51	111.29
4	C	403	S77	C12-C5-C2	2.86	125.64	120.91
4	C	403	S77	C10-C2-C1	2.74	119.91	117.22
4	C	403	S77	C8-C6-N1	-2.74	104.72	110.92
4	B	403	S77	C6-N1-C7	2.71	117.67	111.57
4	A	403	S77	C18-N2-C4	-2.61	125.75	127.78
4	A	403	S77	C15-C14-N3	-2.38	119.66	123.42
4	C	403	S77	C7-C9-C3	-2.37	106.78	110.54
4	C	403	S77	C15-C14-N3	-2.33	119.73	123.42
4	B	403	S77	C7-C9-C3	2.31	114.20	110.54
4	A	403	S77	F-C16-C17	-2.27	116.60	118.66
4	A	403	S77	C9-C3-C4	-2.23	108.44	111.29
4	C	403	S77	C2-C1-N3	-2.17	119.15	122.71
4	C	403	S77	F-C16-C17	2.01	120.48	118.66

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	S77	N3-C1-N1-C6
4	C	403	S77	N3-C1-N1-C7
5	B	406	EDO	O1-C1-C2-O2
4	B	403	S77	C2-C1-N1-C6
4	A	403	S77	N3-C1-N1-C7
5	B	410	EDO	O1-C1-C2-O2
5	C	409	EDO	O1-C1-C2-O2
4	C	403	S77	C2-C1-N1-C7
4	A	403	S77	C2-C1-N1-C7
5	B	409	EDO	O1-C1-C2-O2
5	C	408	EDO	O1-C1-C2-O2
5	A	407	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	412	EDO	O1-C1-C2-O2
4	B	403	S77	C8-C3-C4-N2

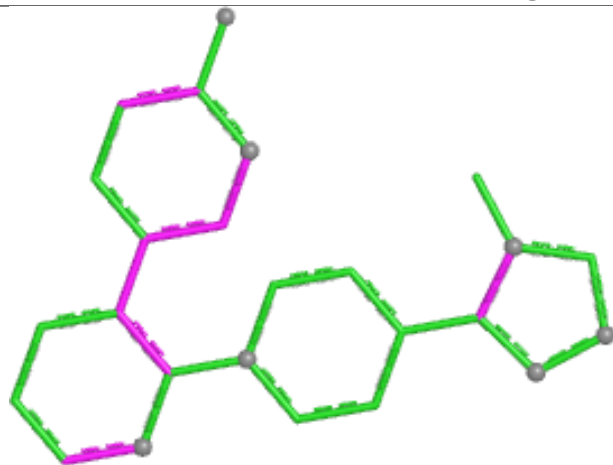
There are no ring outliers.

3 monomers are involved in 3 short contacts:

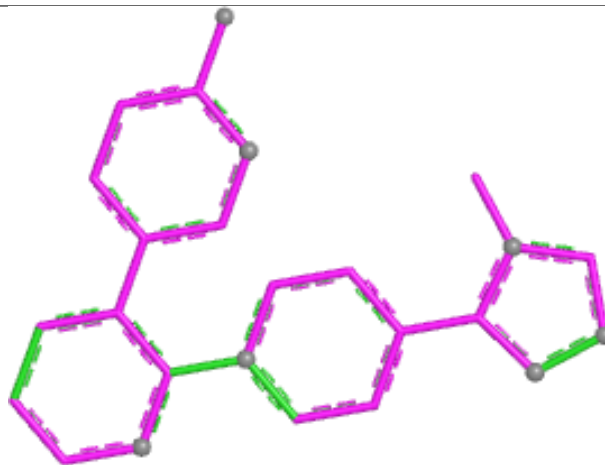
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	412	EDO	1	0
5	C	409	EDO	1	0
5	B	408	EDO	1	0

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

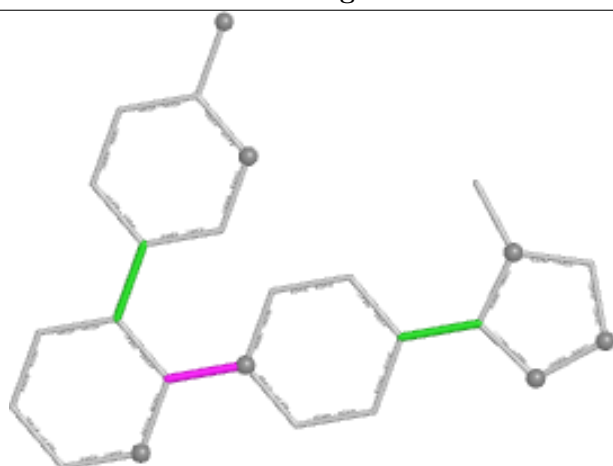
Ligand S77 C 403



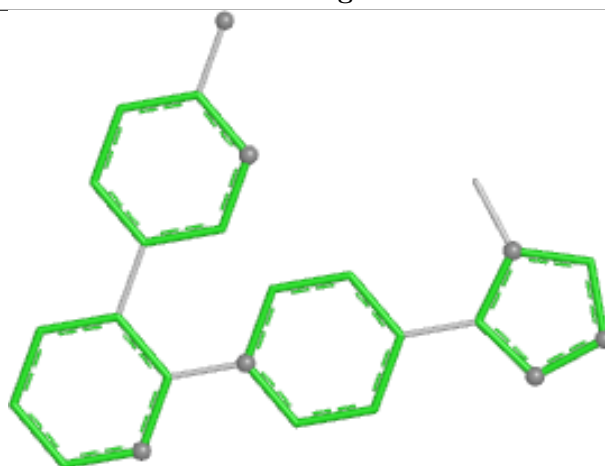
Bond lengths



Bond angles

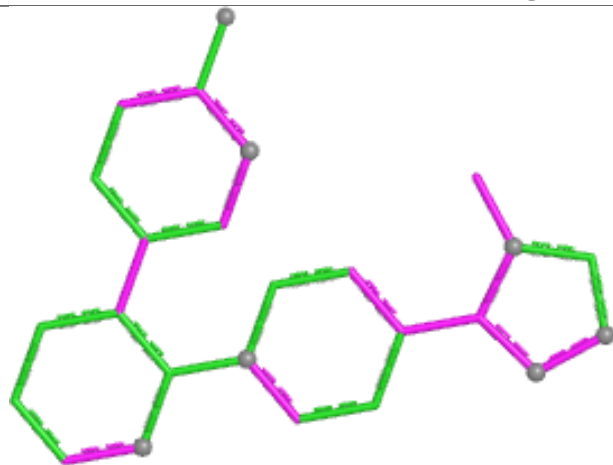


Torsions

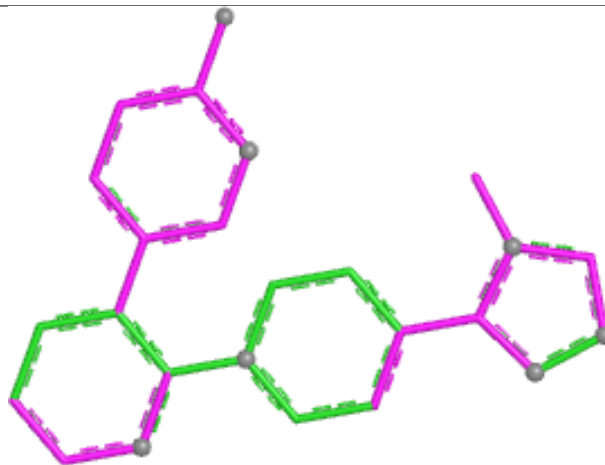


Rings

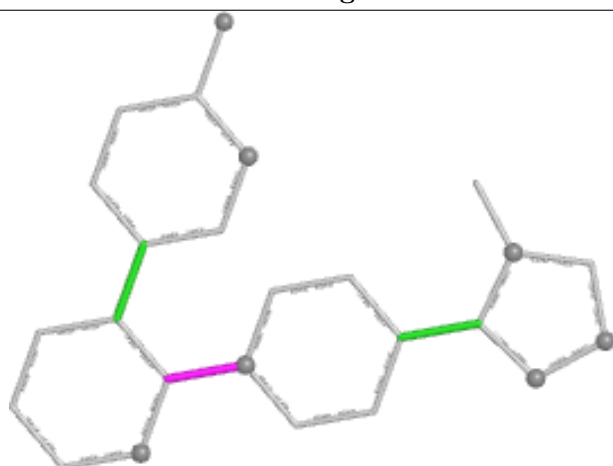
Ligand S77 A 403



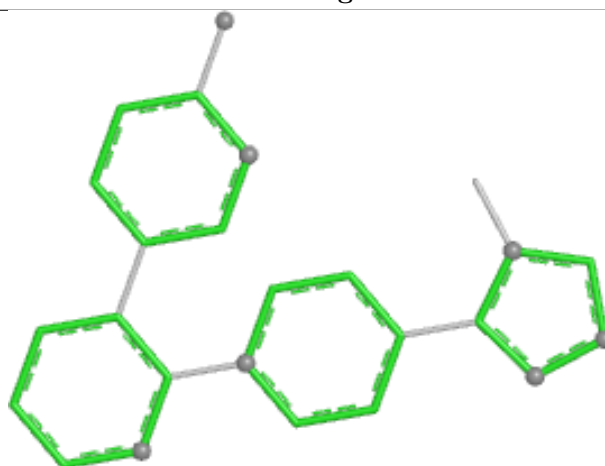
Bond lengths



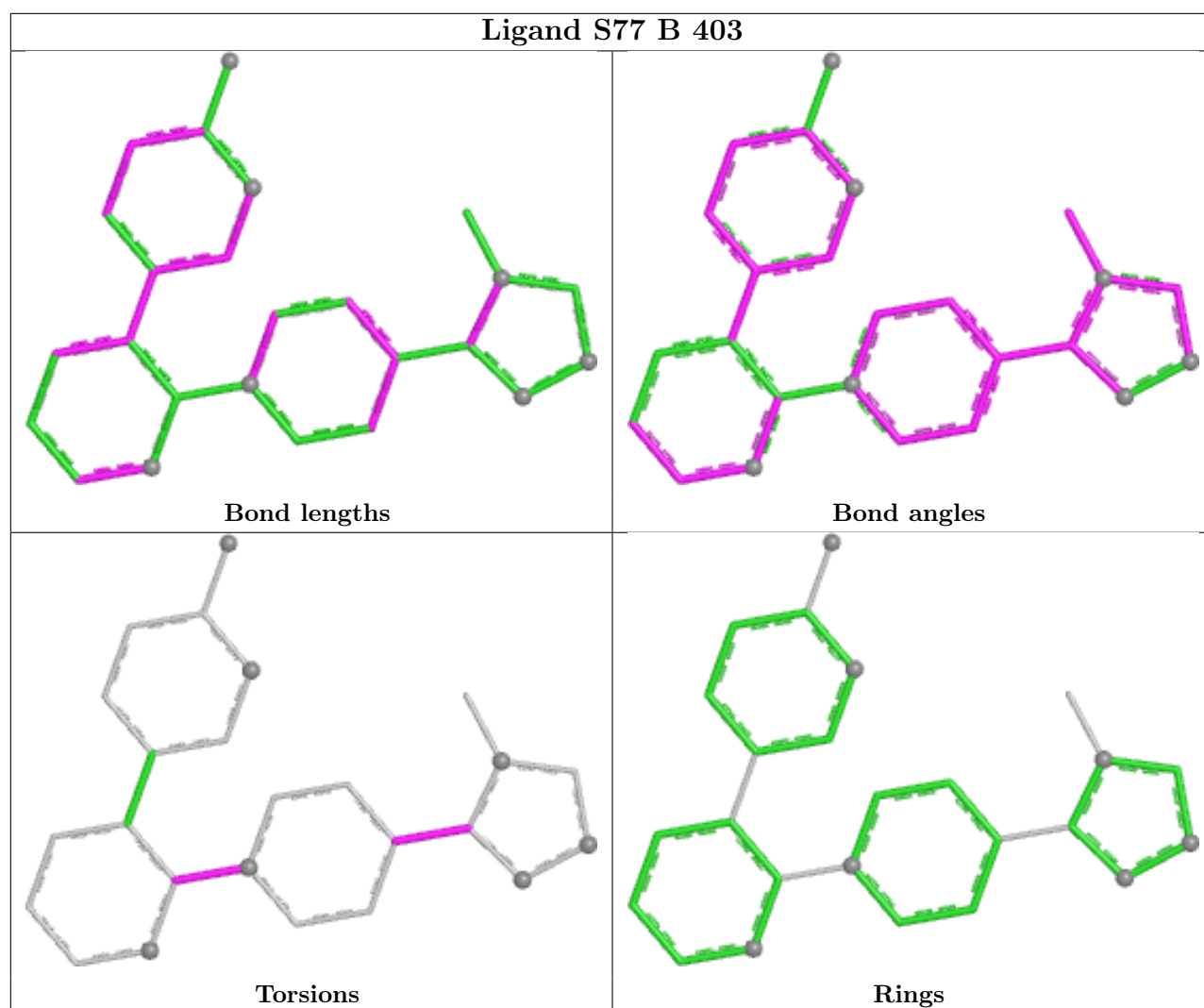
Bond angles



Torsions



Rings



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	328/329 (99%)	-0.19	15 (4%)	37 44	6, 14, 31, 89	2 (0%)
1	B	328/329 (99%)	-0.28	14 (4%)	40 46	7, 13, 29, 83	7 (2%)
1	C	328/329 (99%)	-0.24	14 (4%)	40 46	6, 13, 29, 83	3 (0%)
All	All	984/987 (99%)	-0.24	43 (4%)	39 46	6, 13, 31, 89	12 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	TRP	10.0
1	B	149	TRP	9.3
1	C	149	TRP	9.1
1	C	151	ASN	5.0
1	A	151	ASN	5.0
1	B	151	ASN	4.9
1	A	150	ASN	4.7
1	B	150	ASN	4.5
1	C	150	ASN	4.3
1	A	186	ASP	4.1
1	A	188	LYS	3.9
1	C	184	VAL	3.7
1	C	145	TYR	3.6
1	A	34	SER	3.5
1	C	186	ASP	3.5
1	B	145	TYR	3.4
1	B	186	ASP	3.2
1	B	34	SER	3.2
1	A	145	TYR	3.2
1	C	148	HIS	3.2
1	B	184	VAL	3.0
1	C	187	SER	2.9
1	A	148	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	148	HIS	2.9
1	B	188	LYS	2.8
1	C	34	SER	2.8
1	A	147	SER	2.8
1	C	147	SER	2.6
1	A	300	GLY	2.6
1	A	185	SER	2.6
1	C	35	ALA	2.6
1	A	35	ALA	2.6
1	B	185	SER	2.5
1	A	184	VAL	2.5
1	B	187	SER	2.5
1	C	300	GLY	2.4
1	A	187	SER	2.4
1	C	146	PHE	2.3
1	B	147	SER	2.2
1	B	300	GLY	2.2
1	A	146	PHE	2.2
1	C	185	SER	2.0
1	B	206[A]	HIS	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	EDO	A	408	4/4	0.86	0.16	32,33,37,38	0
5	EDO	A	407	4/4	0.87	0.15	32,36,36,36	0
5	EDO	B	404	4/4	0.88	0.15	32,32,35,36	0

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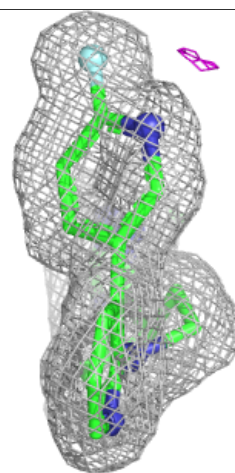
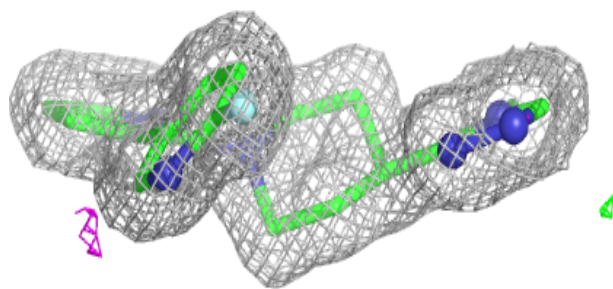
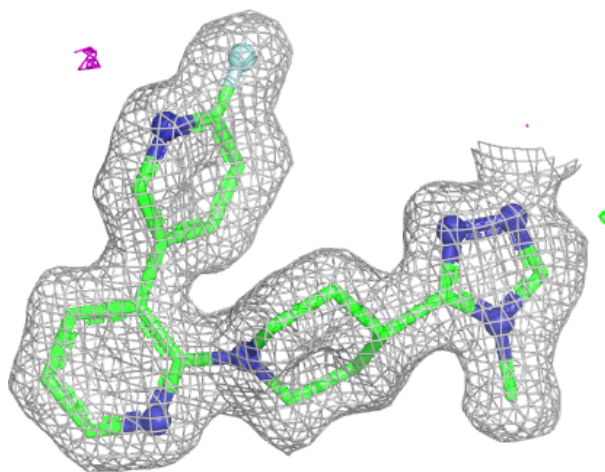
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	410	4/4	0.88	0.14	38,38,40,40	0
5	EDO	B	412	4/4	0.88	0.15	36,37,39,40	0
5	EDO	C	405	4/4	0.88	0.14	29,30,30,35	0
5	EDO	C	407	4/4	0.88	0.12	25,27,28,28	0
5	EDO	C	409	4/4	0.89	0.14	33,36,40,49	0
5	EDO	B	406	4/4	0.90	0.12	30,33,35,37	0
5	EDO	A	405	4/4	0.90	0.10	23,23,23,24	0
5	EDO	B	411	4/4	0.91	0.10	23,25,25,26	0
5	EDO	B	408	4/4	0.92	0.11	28,28,28,29	0
5	EDO	C	406	4/4	0.92	0.12	32,33,34,35	0
5	EDO	C	408	4/4	0.93	0.09	23,24,24,24	0
5	EDO	B	409	4/4	0.93	0.10	32,33,33,33	0
5	EDO	B	407	4/4	0.94	0.09	26,26,27,28	0
5	EDO	A	404	4/4	0.95	0.08	22,22,23,24	0
4	S77	A	403	25/25	0.97	0.05	11,15,17,18	0
4	S77	B	403	25/25	0.97	0.06	12,14,17,18	0
5	EDO	A	406	4/4	0.97	0.06	14,15,15,15	0
5	EDO	B	405	4/4	0.97	0.05	13,13,13,14	0
5	EDO	C	404	4/4	0.98	0.05	12,12,12,13	0
4	S77	C	403	25/25	0.98	0.05	10,14,19,19	0
3	SO4	C	402	5/5	0.99	0.04	13,15,16,17	0
3	SO4	A	402	5/5	0.99	0.05	13,14,17,18	0
3	SO4	B	402	5/5	0.99	0.03	14,14,15,16	0
2	ZN	C	401	1/1	1.00	0.02	12,12,12,12	0
2	ZN	A	401	1/1	1.00	0.02	12,12,12,12	0
2	ZN	B	401	1/1	1.00	0.02	12,12,12,12	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.

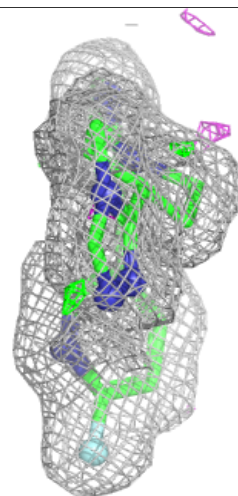
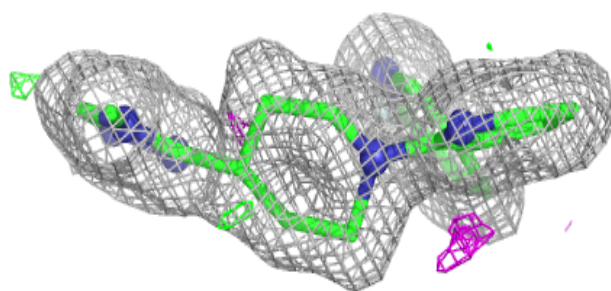
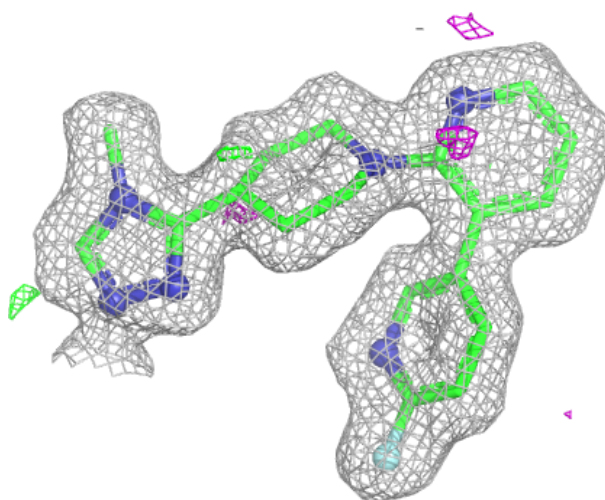
Electron density around S77 A 403:

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



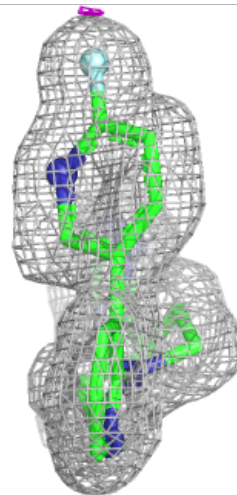
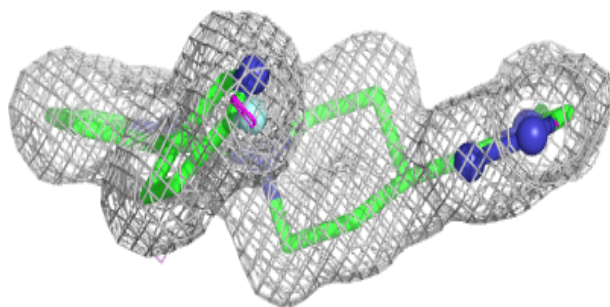
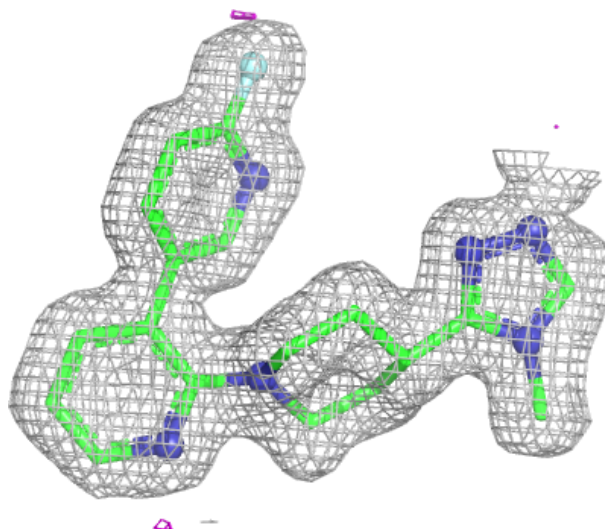
Electron density around S77 B 403:

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



Electron density around S77 C 403:

$2mF_o-DF_c$ (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.