W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2021 – 10:08 am GMT

PDB ID	:	7OYX
Title	:	E.coli's putrescine receptor variant PotF/D (4JDF) with mutations E39D Y87S F88Y S247D in complex with spermidine
Authors	:	Shanmugaratnam, S.; Kroeger, P.; Hocker, B.
Deposited on	:	2021-06-25
Resolution	:	1.37 Å(reported)

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

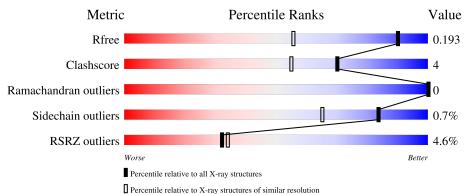|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.37 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	Percentile Ranks	Value
Rfree		0.193
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0.7%
RSRZ outliers		4.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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 <=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	352	4% / 91% / 7% ••
1	B	352	5% / 93% / 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	3IE	A	403	-	-	-	X

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 12500 atoms, of which 5861 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 Putrescine-binding periplasmic protein PotF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	347	Total 5754	C 1858	H 2876	N 479	O 531	S 10	0	22	0
1	B	347	Total 5648	C 1827	H 2808	N 470	O 532	S 11	0	19	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	THR	SER	engineered mutation	UNP P31133
A	88	TYR	PHE	engineered mutation	UNP P31133
A	182	ASP	ALA	engineered mutation	UNP P31133
A	276	TRP	PHE	engineered mutation	UNP P31133
A	348	GLN	LEU	engineered mutation	UNP P31133
A	371	LEU	-	expression tag	UNP P31133
A	372	GLU	-	expression tag	UNP P31133
A	373	HIS	-	expression tag	UNP P31133
A	374	HIS	-	expression tag	UNP P31133
A	375	HIS	-	expression tag	UNP P31133
A	376	HIS	-	expression tag	UNP P31133
A	377	HIS	-	expression tag	UNP P31133
A	378	HIS	-	expression tag	UNP P31133
B	38	THR	SER	engineered mutation	UNP P31133
B	88	TYR	PHE	engineered mutation	UNP P31133
B	182	ASP	ALA	engineered mutation	UNP P31133
B	276	TRP	PHE	engineered mutation	UNP P31133
B	348	GLN	LEU	engineered mutation	UNP P31133
B	371	LEU	-	expression tag	UNP P31133
B	372	GLU	-	expression tag	UNP P31133
B	373	HIS	-	expression tag	UNP P31133
B	374	HIS	-	expression tag	UNP P31133
B	375	HIS	-	expression tag	UNP P31133
B	376	HIS	-	expression tag	UNP P31133
B	377	HIS	-	expression tag	UNP P31133

WORLDWIDE
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PROTEIN DATA BANK

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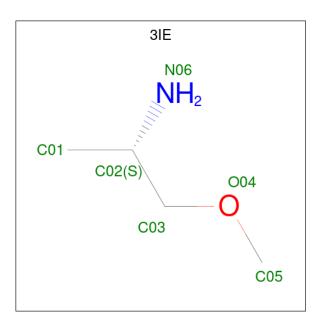| Chain	Residue	Modelled	Actual	Comment	Reference
B	378	HIS	-	expression tag	UNP P31133

- Molecule 2 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 29	C 7	H 19	N 3	0	0
2	B	1	Total 29	C 7	H 19	N 3	0	0

- Molecule 3 is (2 {S})-1-methoxypropan-2-amine (three-letter code: 3IE) (formula: $C_4H_{11}NO$).

3IE

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			17	4	11	1	1		
3	A	1	Total	C	H	N	O	0	0
			17	4	11	1	1		
3	B	1	Total	C	H	N	O	0	0
			17	4	11	1	1		
3	B	1	Total	C	H	N	O	0	0
			17	4	11	1	1		
3	B	1	Total	C	H	N	O	0	0
			17	4	11	1	1		

- Molecule 4 is (2 {S})-1-[(2 {R})-1-(2-methoxyethoxy)propan-2-yl]oxypropan-2-amine (three-letter code: 4SW) (formula: $C_9H_{21}NO_3$).
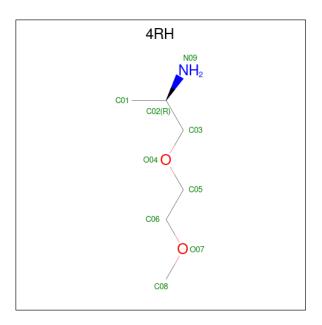
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			34	9	21	1	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	1
			3	3		
5	B	1	Total	Cl	0	1
			2	2		

- Molecule 6 is (2 {R})-1-(2-methoxyethoxy)propan-2-amine (three-letter code: 4RH) (formula: $C_6H_{15}NO_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	0	0
			24	6	15	1	2		

- Molecule 7 is (2 {R})-1-[(2 {R})-1-[(2 {S})-1-[(2 {S})-1-(2-methoxyethoxy)propan-2-yl]oxypropan-2-yl]oxypropan-2-yl]oxypropan-2-amine (three-letter code: 3IK) (formula: $C_{15}H_{33}NO_5$).
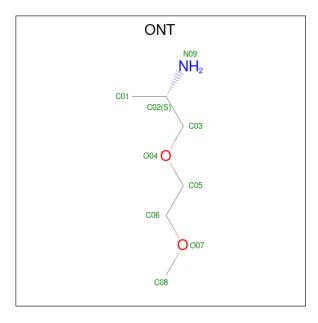

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	0	0
			54	15	33	1	5		

- Molecule 8 is (2 {S})-1-(2-methoxyethoxy)propan-2-amine (three-letter code: ONT)

(formula: $C_6H_{15}NO_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 24	C 6	H 15	N 1	O 2	0	0

- Molecule 9 is water.

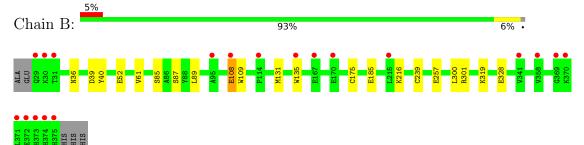| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	390	Total 420	O 420	0	29
9	B	376	Total 394	O 394	0	17

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: Putrescine-binding periplasmic protein PotF

• Molecule 1: Putrescine-binding periplasmic protein PotF

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	117.16Å 71.49Å 92.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.70 – 1.37 45.31 – 1.37	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.70-1.37) 99.8 (45.31-1.37)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 1.37Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.165 , 0.193 0.166 , 0.193	Depositor DCC
R_{free} test set	2099 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	12500	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ONT, 4SW, CL, 4RH, 3IE, 3IK, SPD

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	0.82	0/3034	0.90	3/4130 (0.1%)
1	B	0.77	1/2969 (0.0%)	0.84	0/4041
All	All	0.80	1/6003 (0.0%)	0.87	3/8171 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	GLU	CD-OE2	-5.15	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	298	TYR	CB-CG-CD2	5.80	124.48	121.00
1	A	254	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	40	TYR	CB-CG-CD1	5.01	124.00	121.00

There are no chirality outliers.

There are no planarity outliers.

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	2878	2876	2872	21	0
1	B	2840	2808	2802	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	19	19	2	0
2	B	10	19	19	1	0
3	A	12	22	0	0	0
3	B	18	33	0	0	0
4	A	13	21	0	1	0
5	A	3	0	0	2	0
5	B	2	0	0	0	0
6	B	9	15	0	1	0
7	B	21	33	0	0	0
8	B	9	15	0	0	0
9	A	420	0	0	10	2
9	B	394	0	0	11	2
All	All	6639	5861	5712	41	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 4.

The worst 5 of 41 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:298:TYR:OH	9:A:753[B]:HOH:O	1.82	0.97
1:A:107:PRO:O	9:A:765[B]:HOH:O	1.85	0.94
1:B:52[A]:GLU:OE2	9:B:501:HOH:O	1.85	0.94
5:A:405[B]:CL:CL	9:A:764[B]:HOH:O	2.25	0.92
1:A:340:ASP:OD2	9:A:501:HOH:O	1.87	0.91

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)
9:A:713:HOH:O	9:A:718:HOH:O[2_575]	2.13	0.07
9:B:526:HOH:O	9:B:842:HOH:O[2_565]	2.16	0.04
9:A:855:HOH:O	9:B:819:HOH:O[4_554]	2.18	0.02

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	370/352 (105%)	364 (98%)	6 (2%)	0	100	100
1	B	364/352 (103%)	357 (98%)	7 (2%)	0	100	100
All	All	734/704 (104%)	721 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/299 (107%)	319 (100%)	1 (0%)	92	82
1	B	313/299 (105%)	309 (99%)	4 (1%)	69	41
All	All	633/598 (106%)	628 (99%)	5 (1%)	84	61

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	TYR
1	B	40	TYR
1	B	89	LEU
1	B	108[A]	GLU
1	B	108[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.
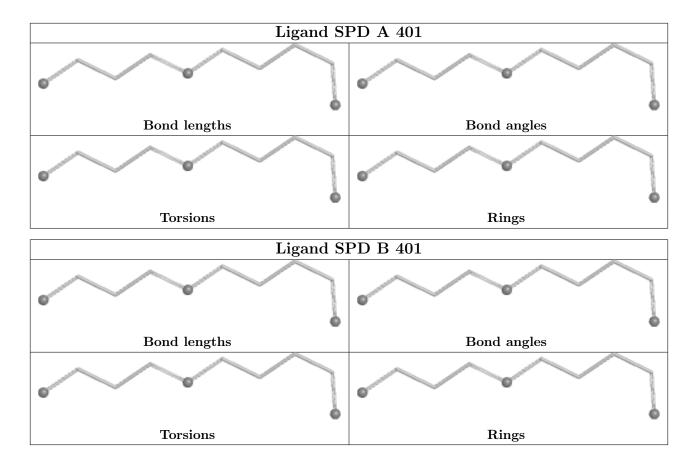
There are no chirality outliers.

There are no torsion outliers.

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 then 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 SPD A 401	
Bond lengths	Bond angles
Torsions	Rings

Ligand SPD B 401	
Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	347/352 (98%)	0.51	13 (3%)	41	44	10, 18, 35, 89	0
1	B	347/352 (98%)	0.53	19 (5%)	25	25	13, 21, 39, 82	0
All	All	694/704 (98%)	0.52	32 (4%)	32	34	10, 19, 38, 89	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	LEU	11.0
1	B	371	LEU	8.0
1	B	369[A]	GLY	7.8
1	A	369	GLY	7.4
1	A	372	GLU	5.6

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.
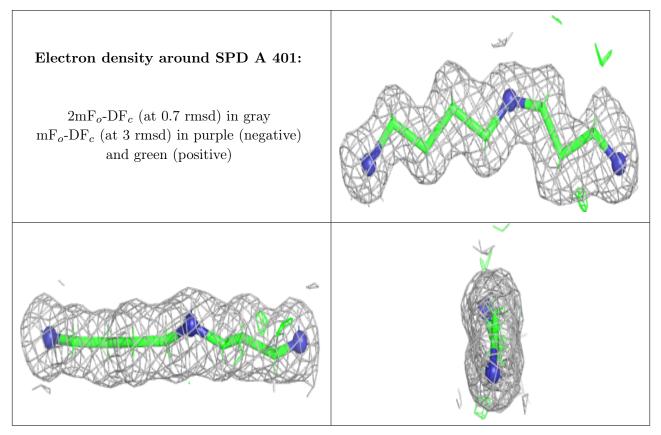
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
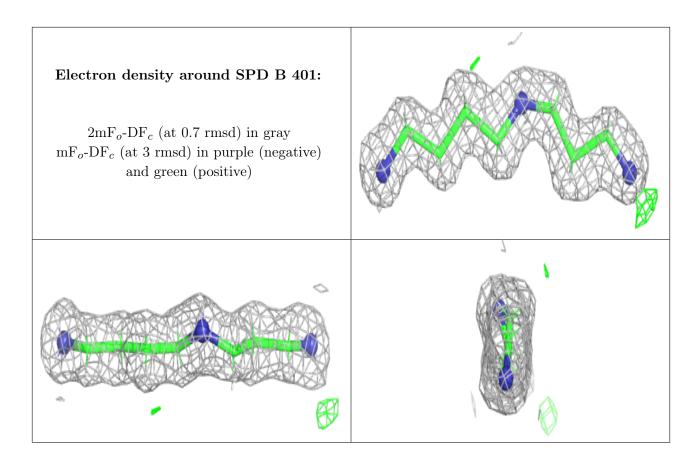
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	3IE	B	405	6/6	0.29	0.24	44,58,63,69	0
3	3IE	A	403	6/6	0.58	0.46	50,64,78,78	0
8	ONT	B	407	9/9	0.68	0.26	52,63,71,71	0
7	3IK	B	403	21/21	0.69	0.17	33,55,70,75	0
4	4SW	A	404	13/13	0.73	0.14	39,63,77,87	0
6	4RH	B	402	9/9	0.73	0.16	33,49,67,67	0
3	3IE	A	402	6/6	0.84	0.15	32,54,71,71	0
5	CL	A	406	1/1	0.86	0.09	58,58,58,58	0
3	3IE	B	404	6/6	0.89	0.30	36,55,89,89	0
3	3IE	B	406	6/6	0.92	0.20	17,34,81,89	0
2	SPD	A	401	10/10	0.94	0.11	11,15,31,37	0
2	SPD	B	401	10/10	0.94	0.09	14,18,28,30	0
5	CL	B	408[B]	1/1	0.99	0.07	16,16,16,16	1
5	CL	A	405[B]	1/1	0.99	0.11	18,18,18,18	1
5	CL	A	405[A]	1/1	0.99	0.11	16,16,16,16	1
5	CL	B	408[A]	1/1	0.99	0.07	18,18,18,18	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 SPD A 401:

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

Electron density around SPD B 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.