



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 PM UTC

PDB ID : 7ZCY / pdb_00007zcy
Title : Sporosarcina pasteurii urease (SPU) co-crystallized in the presence of an Ebselen-derivative and bound to Se atoms
Authors : Mazzei, L.; Ciurli, S.; Cianci, M.
Deposited on : 2022-03-29
Resolution : 1.54 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

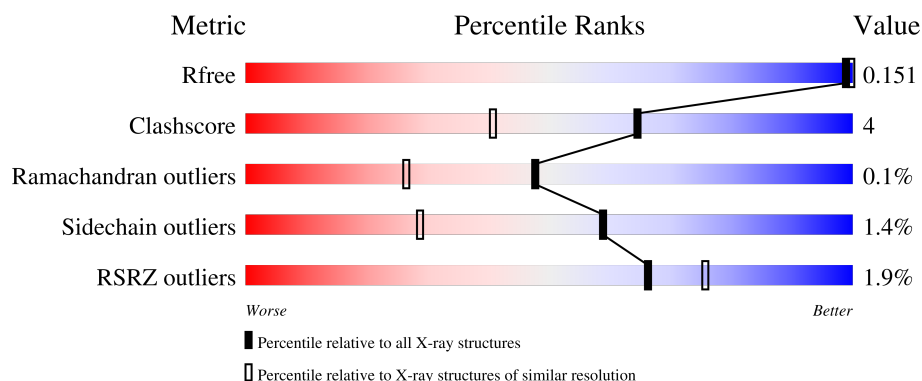
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	100	2% 89% 9% .
2	B	122	2% 88% 12% .
3	C	570	2% 91% 8% .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7282 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	9	0
			853	535	145	164	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	LEU	variant	UNP P41022
A	22	LYS	ARG	variant	UNP P41022

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	7	0
			1015	625	185	204	1			

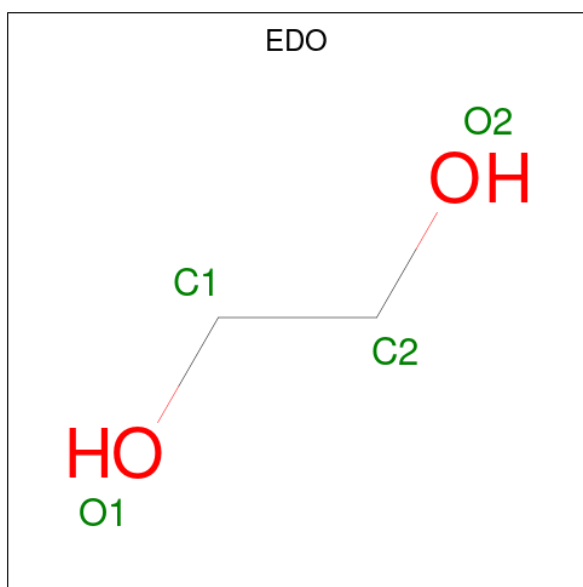
- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	570	Total	C	N	O	S	0	25	0
			4504	2825	780	871	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	35	TYR	-	insertion	UNP P41020
C	?	-	VAL	deletion	UNP P41020

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



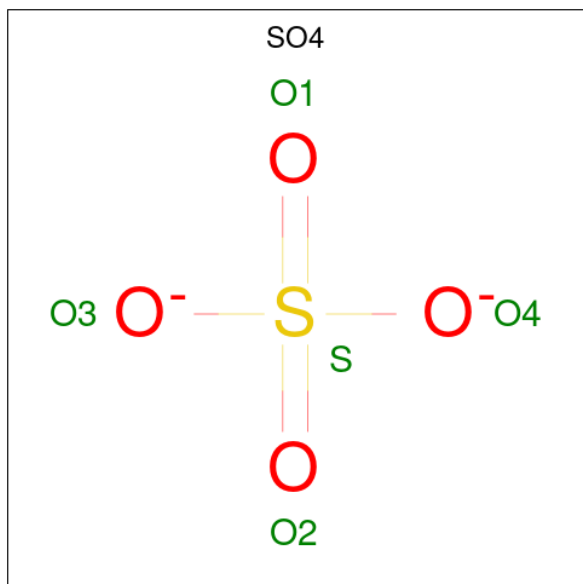
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

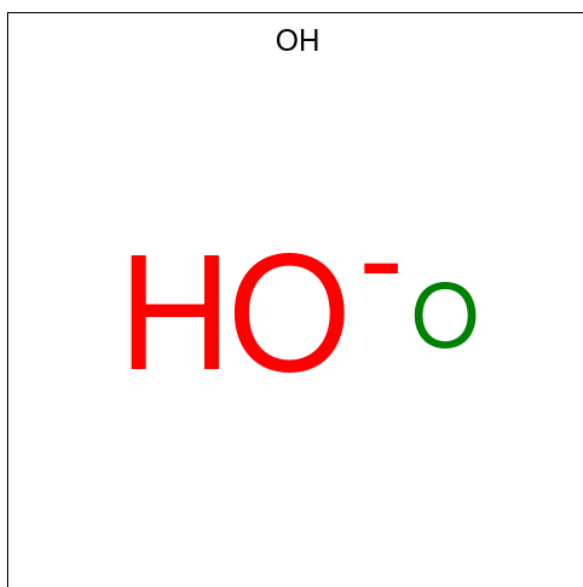
Continued from previous page...

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

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

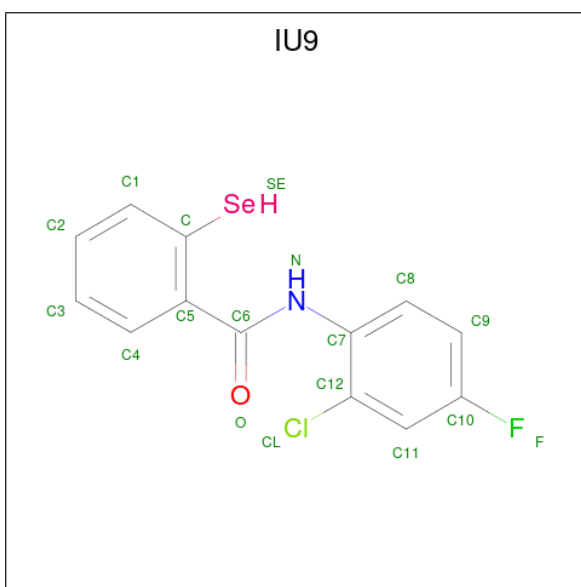
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	Ni	0	0
			2	2		

- Molecule 7 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	O	0	0
			1	1		

- Molecule 8 is N-(2-chloranyl-4-fluoranyl-phenyl)-2-selanyl-benzamide (CCD ID: IU9) (formula: C₁₃H₉ClFNOSe) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	Cl	F	N	O	Se	
			18	13	1	1	1	1	1	0

- Molecule 9 is SELENIUM ATOM (CCD ID: SE) (formula: Se).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	2	Total	Se		
			2	2	0	0

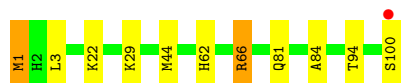
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	100	Total	O		
			100	100	0	0
10	B	172	Total	O		
			172	172	0	0
10	C	495	Total	O		
			495	495	0	0

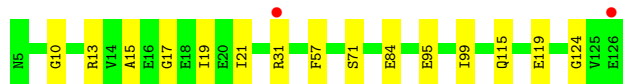
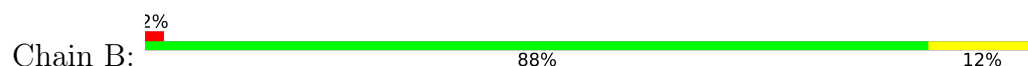
3 Residue-property plots [i](#)

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.

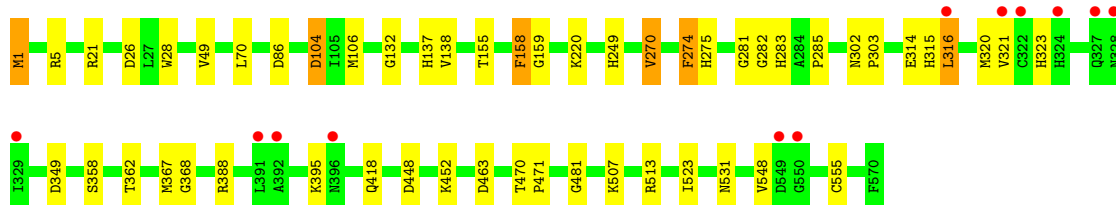
- Molecule 1: Urease subunit gamma



- Molecule 2: Urease subunit beta



- Molecule 3: Urease subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.61Å 131.61Å 189.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.80 – 1.54 97.80 – 1.54	Depositor EDS
% Data completeness (in resolution range)	100.0 (97.80-1.54) 100.0 (97.80-1.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.137 , 0.160 (Not available) , 0.151	Depositor DCC
R_{free} test set	7018 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7282	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, EDO, OH, CXM, SE, IU9, KCX, SO4

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	0.99	0/849	1.04	0/1140
2	B	0.99	0/1027	1.06	0/1379
3	C	1.05	2/4593 (0.0%)	1.14	7/6218 (0.1%)
All	All	1.04	2/6469 (0.0%)	1.12	7/8737 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	448	ASP	CG-OD1	-5.31	1.15	1.25
3	C	315	HIS	CE1-NE2	5.11	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	104	ASP	CA-CB-CG	8.30	120.90	112.60
3	C	349	ASP	CA-CB-CG	5.33	117.93	112.60
3	C	274	PHE	CA-CB-CG	5.24	119.04	113.80
3	C	548	VAL	CA-C-O	-5.15	115.04	120.39
3	C	463	ASP	CA-CB-CG	5.13	117.73	112.60
3	C	316	LEU	N-CA-C	-5.08	105.63	111.07
3	C	26	ASP	CA-CB-CG	5.00	117.60	112.60

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	853	0	865	8	0
2	B	1015	0	993	12	0
3	C	4504	0	4484	37	0
4	A	20	0	30	0	0
4	C	60	0	90	6	0
5	A	5	0	0	0	0
5	B	15	0	0	0	0
5	C	20	0	0	0	0
6	C	2	0	0	0	0
7	C	1	0	0	0	0
8	C	18	0	0	2	0
9	C	2	0	0	0	0
10	A	100	0	0	4	0
10	B	172	0	0	0	0
10	C	495	0	0	8	0
All	All	7282	0	6462	51	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 4.

All (51) 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)
3:C:555:CYS:SG	8:C:605:IU9:SE	2.42	1.27
8:C:605:IU9:SE	8:C:605:IU9:O	2.14	1.15
3:C:303[B]:PRO:HG2	10:C:1088:HOH:O	1.86	0.74
3:C:270[B]:VAL:HG12	10:C:860:HOH:O	1.87	0.73
3:C:270[B]:VAL:HG11	3:C:523:ILE:O	1.91	0.71
2:B:17:GLY:O	3:C:5[A]:ARG:HG2	1.92	0.69
2:B:115:GLN:O	2:B:119[A]:GLU:HG3	1.92	0.69
1:A:1[B]:CXM:HE3	1:A:3:LEU:HD21	1.78	0.66
3:C:507[C]:LYS:NZ	10:C:704:HOH:O	2.29	0.64
2:B:21:ILE:HD11	3:C:1[A]:MET:HG2	1.79	0.64
4:C:610:EDO:H12	10:C:1108:HOH:O	2.02	0.59
3:C:513[B]:ARG:NE	4:C:620:EDO:O2	2.35	0.57
3:C:388[B]:ARG:NH2	4:C:617:EDO:O1	2.40	0.55
2:B:21:ILE:CD1	3:C:1[A]:MET:HG2	2.36	0.54
3:C:507[C]:LYS:CE	10:C:704:HOH:O	2.56	0.54
2:B:13[A]:ARG:HG3	3:C:28:TRP:CZ3	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:316:LEU:O	3:C:320:MET:HG2	2.08	0.54
1:A:29[B]:LYS:NZ	10:A:303:HOH:O	2.41	0.53
2:B:95:GLU:O	3:C:104:ASP:HB3	2.10	0.52
3:C:249:HIS:CE1	3:C:281:GLY:HA3	2.45	0.51
1:A:62:HIS:HD2	10:A:389:HOH:O	1.92	0.51
3:C:303[B]:PRO:HG3	3:C:367:MET:O	2.12	0.50
4:C:622:EDO:H22	10:C:803:HOH:O	2.11	0.50
3:C:132:GLY:HA3	3:C:155:THR:OG1	2.12	0.49
3:C:513[B]:ARG:NH2	4:C:620:EDO:O2	2.45	0.48
2:B:15:ALA:O	3:C:5[B]:ARG:HD2	2.14	0.48
3:C:362:THR:O	3:C:368:GLY:HA3	2.14	0.47
3:C:302:ASN:N	3:C:303[B]:PRO:CD	2.78	0.47
3:C:323:HIS:CE1	4:C:604:EDO:H11	2.51	0.46
3:C:158:PHE:CE2	3:C:418[A]:GLN:CG	2.98	0.45
1:A:22:LYS:HE2	10:A:382:HOH:O	2.16	0.45
3:C:282:GLY:O	3:C:283:HIS:C	2.60	0.45
3:C:138:VAL:O	3:C:159:GLY:HA3	2.17	0.44
2:B:71:SER:OG	3:C:49[A]:VAL:HG21	2.18	0.44
3:C:70:LEU:HD11	3:C:86:ASP:HB3	1.99	0.44
1:A:44[B]:MET:SD	1:A:84:ALA:HB2	2.59	0.43
3:C:274:PHE:O	3:C:275:HIS:C	2.61	0.43
3:C:358:SER:HA	3:C:531:ASN:HB3	2.01	0.43
3:C:49[A]:VAL:HG11	3:C:106:MET:CE	2.49	0.42
1:A:29[A]:LYS:NZ	10:A:306:HOH:O	2.52	0.42
3:C:137:HIS:CE1	3:C:274:PHE:CD2	3.07	0.42
1:A:66[B]:ARG:HD2	1:A:100:SER:O	2.20	0.41
3:C:470:THR:N	3:C:471:PRO:CD	2.84	0.41
2:B:19:ILE:HG12	3:C:5[A]:ARG:HD2	2.03	0.41
2:B:10:GLY:HA2	3:C:21:ARG:O	2.21	0.41
2:B:31[B]:ARG:HG2	2:B:84:GLU:HG2	2.01	0.41
3:C:507[C]:LYS:HE3	10:C:704:HOH:O	2.19	0.41
2:B:57:PHE:O	2:B:124:GLY:HA3	2.20	0.41
3:C:158:PHE:CE2	3:C:418[A]:GLN:HG2	2.57	0.40
1:A:81[B]:GLN:HG2	1:A:94:THR:OG1	2.21	0.40
3:C:481:GLY:HA3	10:C:1052:HOH:O	2.21	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	106/100 (106%)	105 (99%)	1 (1%)	0	100	100
2	B	127/122 (104%)	121 (95%)	5 (4%)	1 (1%)	16	3
3	C	591/570 (104%)	568 (96%)	23 (4%)	0	100	100
All	All	824/792 (104%)	794 (96%)	29 (4%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ILE

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	91/83 (110%)	89 (98%)	2 (2%)	45	15
2	B	108/101 (107%)	108 (100%)	0	100	100
3	C	482/458 (105%)	472 (98%)	10 (2%)	47	16
All	All	681/642 (106%)	669 (98%)	12 (2%)	59	21

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66[A]	ARG
1	A	66[B]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	1[A]	MET
3	C	1[B]	MET
3	C	158	PHE
3	C	270[A]	VAL
3	C	270[B]	VAL
3	C	285	PRO
3	C	314	GLU
3	C	321	VAL
3	C	395	LYS
3	C	452	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	97	ASN
3	C	179	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	KCX	C	220	6,3	10,11,12	0.76	0	6,12,14	1.68	2 (33%)
1	CXM	A	1[B]	1	9,10,11	2.18	1 (11%)	9,11,13	2.13	1 (11%)
1	CXM	A	1[A]	1	9,10,11	1.56	1 (11%)	9,11,13	1.97	1 (11%)

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	KCX	C	220	6,3	-	0/9/10/12	-
1	CXM	A	1[B]	1	-	3/9/10/12	-
1	CXM	A	1[A]	1	-	3/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1[B]	CXM	ON1-CN	6.25	1.33	1.21
1	A	1[A]	CXM	ON1-CN	4.14	1.29	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1[B]	CXM	ON1-CN-N	-5.80	115.34	124.86
1	A	1[A]	CXM	ON1-CN-N	-5.46	115.90	124.86
3	C	220	KCX	OQ1-CX-NZ	-3.09	120.22	124.92
3	C	220	KCX	CE-NZ-CX	2.68	126.53	121.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1[A]	CXM	CB-CA-N-CN
1	A	1[B]	CXM	CB-CA-N-CN
1	A	1[B]	CXM	ON1-CN-N-CA
1	A	1[A]	CXM	C-CA-N-CN
1	A	1[B]	CXM	C-CA-N-CN
1	A	1[A]	CXM	ON1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1[B]	CXM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are monoatomic and 1 is modelled with single atom - leaving 29 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	$\# Z > 2$
4	EDO	A	203	-	3,3,3	0.38	0	2,2,2	0.37	0
4	EDO	C	614	-	3,3,3	0.37	0	2,2,2	0.35	0
4	EDO	C	622	-	3,3,3	0.16	0	2,2,2	0.59	0
4	EDO	C	618	-	3,3,3	0.13	0	2,2,2	0.16	0
4	EDO	C	604	-	3,3,3	0.58	0	2,2,2	0.52	0
5	SO4	B	201	-	4,4,4	0.44	0	6,6,6	0.12	0
4	EDO	A	202	-	3,3,3	0.94	0	2,2,2	0.57	0
4	EDO	C	611	-	3,3,3	0.32	0	2,2,2	0.29	0
4	EDO	C	619	-	3,3,3	0.33	0	2,2,2	0.18	0
4	EDO	C	616	-	3,3,3	0.33	0	2,2,2	0.70	0
5	SO4	C	608	-	4,4,4	0.31	0	6,6,6	0.08	0
8	IU9	C	605	-	18,19,19	3.08	1 (5%)	25,26,26	2.33	3 (12%)
4	EDO	C	610	-	3,3,3	0.49	0	2,2,2	0.42	0
5	SO4	B	202	-	4,4,4	0.25	0	6,6,6	0.26	0
4	EDO	C	621	-	3,3,3	0.20	0	2,2,2	0.19	0
5	SO4	C	609	-	4,4,4	0.30	0	6,6,6	0.07	0
4	EDO	C	613	-	3,3,3	0.06	0	2,2,2	0.05	0
4	EDO	A	206	-	3,3,3	0.53	0	2,2,2	0.66	0
4	EDO	C	617	-	3,3,3	0.24	0	2,2,2	0.36	0
4	EDO	C	612	-	3,3,3	0.22	0	2,2,2	0.39	0
4	EDO	A	205	-	3,3,3	0.67	0	2,2,2	0.38	0
5	SO4	C	606	-	4,4,4	0.30	0	6,6,6	0.38	0
5	SO4	A	204	-	4,4,4	0.47	0	6,6,6	0.18	0
5	SO4	B	203	-	4,4,4	0.34	0	6,6,6	0.07	0
4	EDO	A	201	-	3,3,3	1.07	0	2,2,2	0.59	0
4	EDO	C	615	-	3,3,3	0.48	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	620	-	3,3,3	0.63	0	2,2,2	0.38	0
4	EDO	C	623	-	3,3,3	0.21	0	2,2,2	0.22	0
5	SO4	C	607	-	4,4,4	0.53	0	6,6,6	0.21	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
4	EDO	A	203	-	-	0/1/1/1	-
4	EDO	C	614	-	-	1/1/1/1	-
4	EDO	C	622	-	-	0/1/1/1	-
4	EDO	C	618	-	-	0/1/1/1	-
4	EDO	C	604	-	-	1/1/1/1	-
4	EDO	A	202	-	-	0/1/1/1	-
4	EDO	C	611	-	-	0/1/1/1	-
4	EDO	C	619	-	-	1/1/1/1	-
4	EDO	C	616	-	-	1/1/1/1	-
8	IU9	C	605	-	-	0/8/8/8	0/2/2/2
4	EDO	C	610	-	-	1/1/1/1	-
4	EDO	C	621	-	-	1/1/1/1	-
4	EDO	C	613	-	-	1/1/1/1	-
4	EDO	A	206	-	-	1/1/1/1	-
4	EDO	C	617	-	-	0/1/1/1	-
4	EDO	C	612	-	-	0/1/1/1	-
4	EDO	A	205	-	-	1/1/1/1	-
4	EDO	A	201	-	-	0/1/1/1	-
4	EDO	C	615	-	-	0/1/1/1	-
4	EDO	C	620	-	-	0/1/1/1	-
4	EDO	C	623	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	605	IU9	SE-C	12.98	2.04	1.89

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	605	IU9	C-C5-C6	-10.13	110.23	120.26
8	C	605	IU9	C4-C5-C6	4.12	129.50	118.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	605	IU9	C4-C5-C	2.02	120.23	117.75

There are no chirality outliers.

All (9) torsion outliers are listed below:

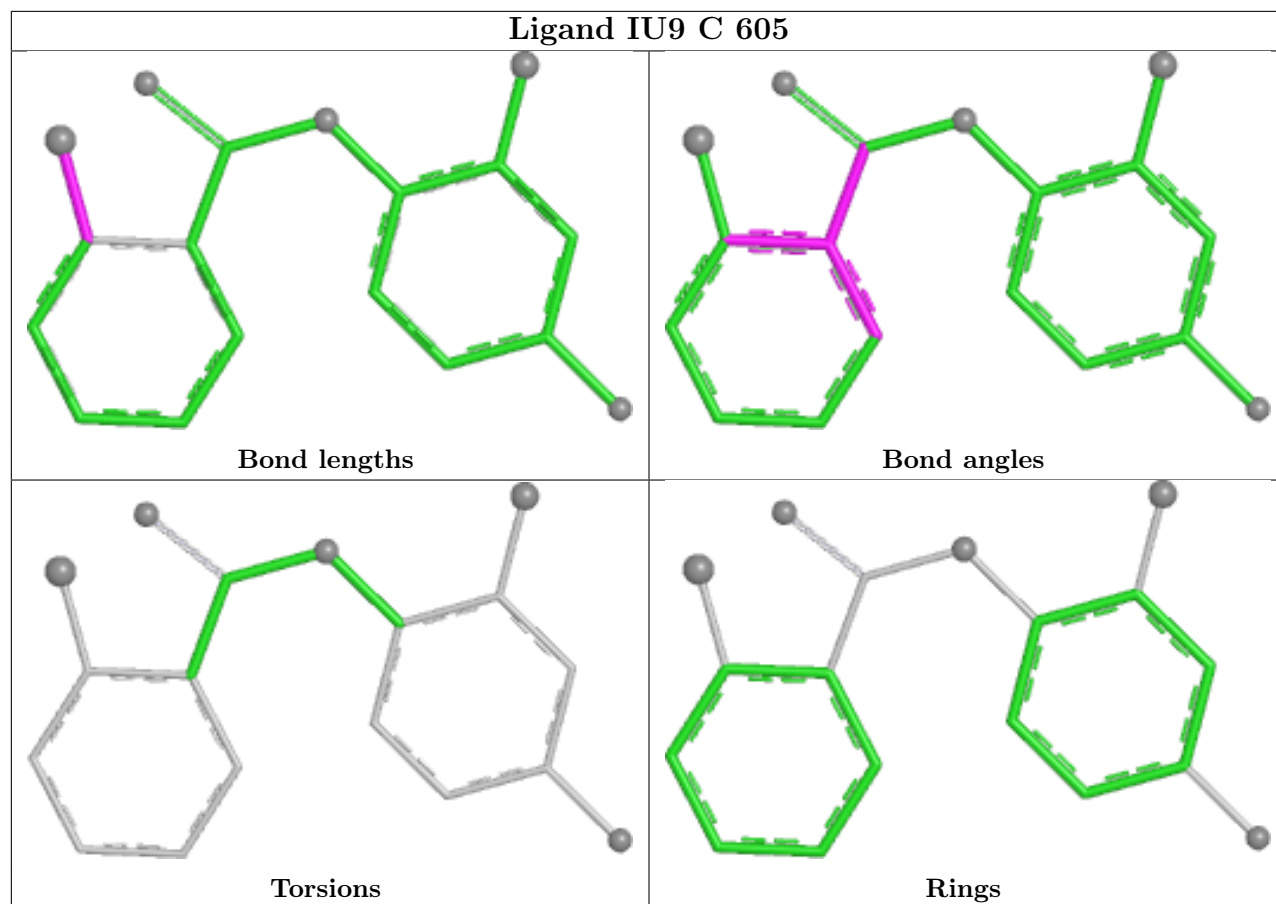
Mol	Chain	Res	Type	Atoms
4	A	206	EDO	O1-C1-C2-O2
4	C	613	EDO	O1-C1-C2-O2
4	C	619	EDO	O1-C1-C2-O2
4	C	610	EDO	O1-C1-C2-O2
4	C	616	EDO	O1-C1-C2-O2
4	A	205	EDO	O1-C1-C2-O2
4	C	614	EDO	O1-C1-C2-O2
4	C	621	EDO	O1-C1-C2-O2
4	C	604	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	622	EDO	1	0
4	C	604	EDO	1	0
8	C	605	IU9	2	0
4	C	610	EDO	1	0
4	C	617	EDO	1	0
4	C	620	EDO	2	0

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



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	99/100 (99%)	-0.29	1 (1%) 79 85	11, 23, 31, 46	8 (8%)
2	B	122/122 (100%)	-0.06	2 (1%) 70 78	12, 25, 37, 62	7 (5%)
3	C	569/570 (99%)	-0.21	12 (2%) 63 73	11, 22, 39, 74	25 (4%)
All	All	790/792 (99%)	-0.20	15 (1%) 66 76	11, 23, 37, 74	40 (5%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	321	VAL	4.3
3	C	322	CYS	4.0
3	C	391	LEU	3.4
3	C	329	ILE	3.2
3	C	550	GLY	3.0
2	B	31[A]	ARG	3.0
3	C	549	ASP	2.9
1	A	100	SER	2.9
3	C	324	HIS	2.8
3	C	327	GLN	2.6
3	C	316	LEU	2.5
3	C	396	ASN	2.5
2	B	126	GLU	2.3
3	C	328	ASN	2.1
3	C	392	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CXM	A	1[A]	11/12	0.98	0.06	22,23,27,29	11
1	CXM	A	1[B]	11/12	0.98	0.06	19,21,23,24	11
3	KCX	C	220	12/13	0.98	0.05	19,20,22,22	0

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.

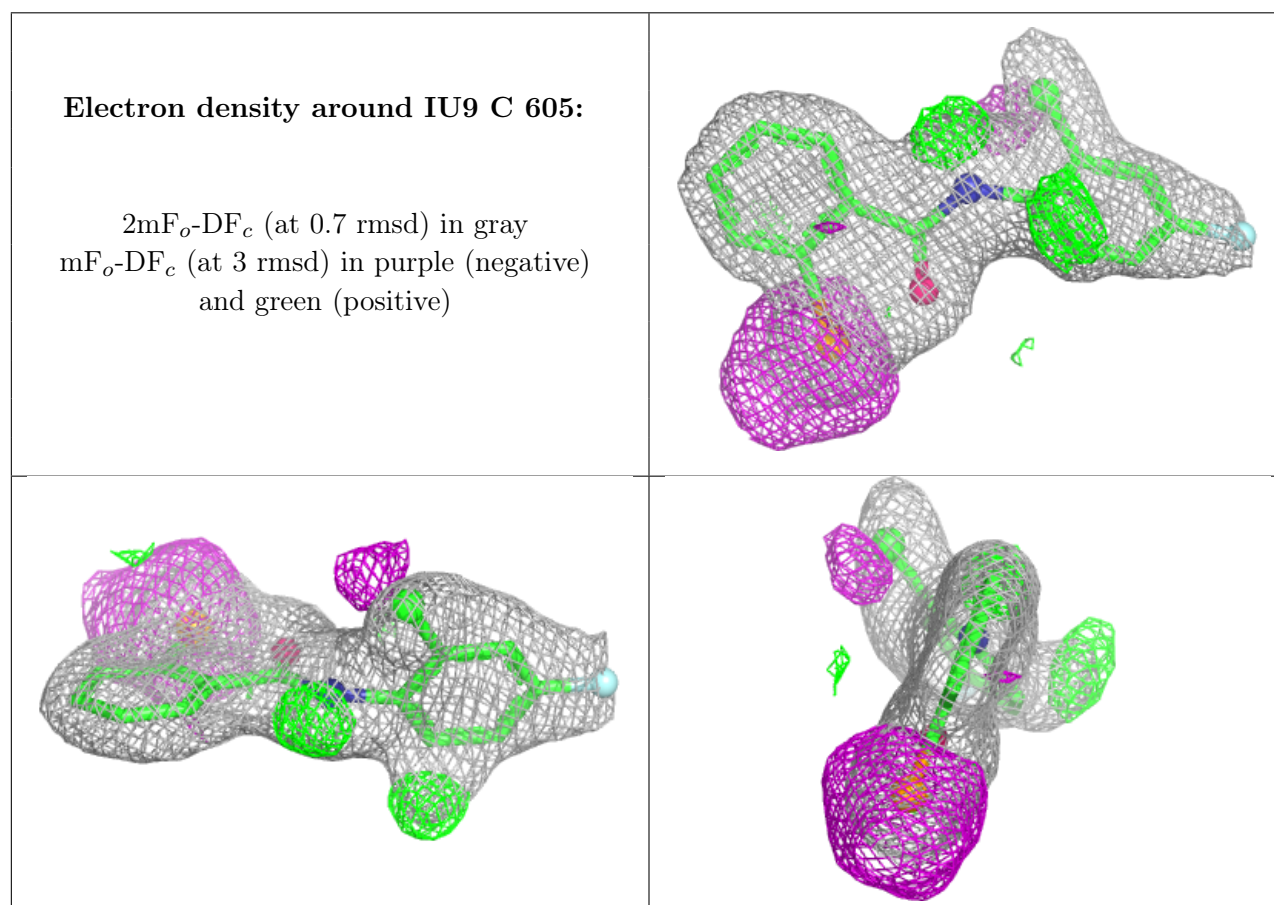
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	B	203	5/5	0.71	0.15	109,111,129,133	0
4	EDO	C	616	4/4	0.72	0.21	60,61,62,65	0
4	EDO	C	622	4/4	0.75	0.20	54,59,62,64	0
4	EDO	C	620	4/4	0.76	0.20	44,48,53,53	0
5	SO4	C	609	5/5	0.76	0.13	88,88,89,92	5
4	EDO	C	619	4/4	0.77	0.16	55,59,61,66	0
5	SO4	B	201	5/5	0.77	0.17	48,53,54,60	5
4	EDO	C	623	4/4	0.78	0.21	55,64,70,75	0
4	EDO	C	613	4/4	0.78	0.19	65,67,68,71	0
4	EDO	A	206	4/4	0.79	0.19	39,41,51,54	0
4	EDO	A	201	4/4	0.81	0.17	37,39,40,40	0
5	SO4	B	202	5/5	0.81	0.10	53,66,76,78	0
5	SO4	C	608	5/5	0.82	0.10	76,86,89,89	5
5	SO4	A	204	5/5	0.83	0.12	46,57,67,79	0
4	EDO	C	604	4/4	0.83	0.18	38,53,57,59	0
4	EDO	C	614	4/4	0.85	0.15	44,45,47,55	0
5	SO4	C	607	5/5	0.85	0.10	46,62,70,77	0
4	EDO	C	621	4/4	0.86	0.15	66,66,66,68	0
9	SE	C	624	1/1	0.86	0.24	82,82,82,82	1
9	SE	C	625	1/1	0.88	0.17	90,90,90,90	1
4	EDO	C	611	4/4	0.89	0.13	38,50,53,57	0
4	EDO	A	205	4/4	0.89	0.10	27,34,36,53	0
4	EDO	C	612	4/4	0.90	0.13	42,45,48,58	0
4	EDO	C	610	4/4	0.90	0.16	41,42,45,64	0
4	EDO	C	618	4/4	0.91	0.11	48,51,52,52	0
4	EDO	A	202	4/4	0.92	0.12	34,35,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	OH	C	603	1/1	0.93	0.09	21,21,21,21	0
4	EDO	C	617	4/4	0.93	0.10	42,50,53,55	0
4	EDO	C	615	4/4	0.93	0.10	32,35,39,39	0
8	IU9	C	605	18/18	0.94	0.13	36,43,75,80	0
5	SO4	C	606	5/5	0.95	0.09	37,38,41,47	5
4	EDO	A	203	4/4	0.96	0.09	26,36,36,37	0
6	NI	C	601	1/1	1.00	0.02	21,21,21,21	0
6	NI	C	602	1/1	1.00	0.03	21,21,21,21	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.