



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:36 PM UTC

PDB ID : 4G8O / pdb_00004g8o
Title : Crystal Structure of a novel small molecule inactivator bound to plasminogen activator inhibitor-1
Authors : Stuckey, J.A.; Lawrence, D.A.; Li, S.-H.
Deposited on : 2012-07-23
Resolution : 2.71 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

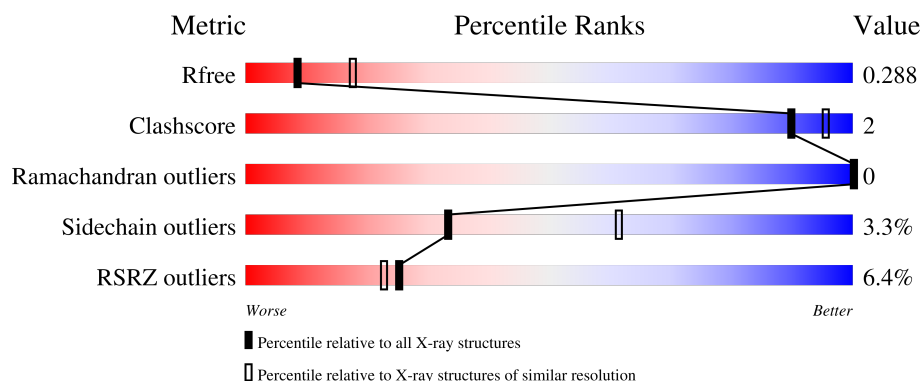
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	376	6% 88% 7% 5%
1	B	376	3% 89% 6% 5%
1	C	376	9% 90% 7% ..
1	D	376	7% 89% 8% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11723 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 Plasminogen activator inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2841	1829	477	521	14			
1	B	359	Total	C	N	O	S	0	0	0
			2851	1835	485	517	14			
1	C	367	Total	C	N	O	S	0	0	0
			2912	1874	495	528	15			
1	D	367	Total	C	N	O	S	0	0	0
			2881	1853	486	527	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	-	expression tag	UNP P05121
A	150	HIS	ASN	engineered mutation	UNP P05121
A	154	THR	LYS	engineered mutation	UNP P05121
A	319	LEU	GLN	engineered mutation	UNP P05121
A	354	ILE	MET	engineered mutation	UNP P05121
B	4	ALA	-	expression tag	UNP P05121
B	150	HIS	ASN	engineered mutation	UNP P05121
B	154	THR	LYS	engineered mutation	UNP P05121
B	319	LEU	GLN	engineered mutation	UNP P05121
B	354	ILE	MET	engineered mutation	UNP P05121
C	4	ALA	-	expression tag	UNP P05121
C	150	HIS	ASN	engineered mutation	UNP P05121
C	154	THR	LYS	engineered mutation	UNP P05121
C	319	LEU	GLN	engineered mutation	UNP P05121
C	354	ILE	MET	engineered mutation	UNP P05121
D	4	ALA	-	expression tag	UNP P05121
D	150	HIS	ASN	engineered mutation	UNP P05121
D	154	THR	LYS	engineered mutation	UNP P05121
D	319	LEU	GLN	engineered mutation	UNP P05121
D	354	ILE	MET	engineered mutation	UNP P05121

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



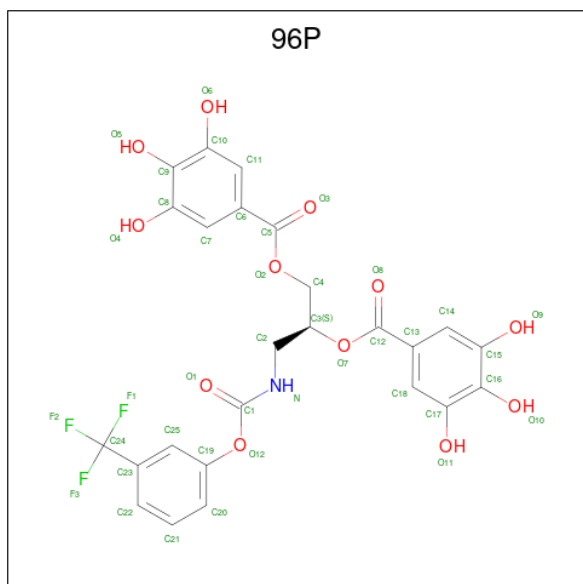
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is (2S)-3-({[3-(trifluoromethyl)phenoxy]carbonyl}amino)propane-1,2-diyl bis(3,4,5-trihydroxybenzoate) (CCD ID: 96P) (formula: C₂₅H₂₀F₃NO₁₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	F	N	O	21	0
			41	25	3	1	12		

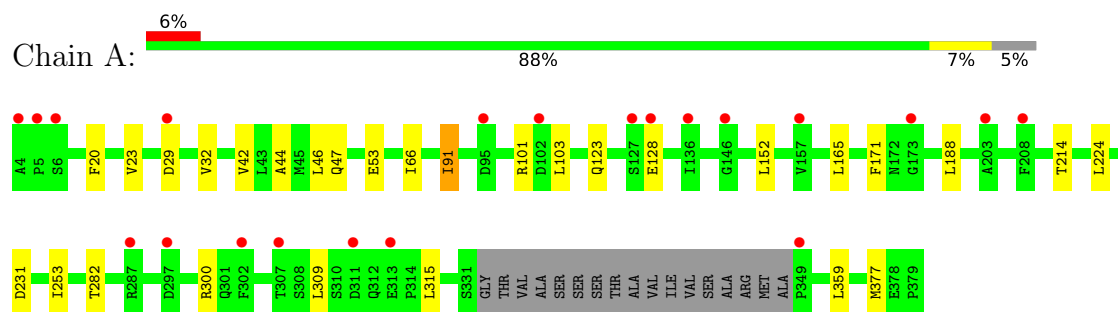
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total 40	O 40	0	0
5	B	46	Total 46	O 46	0	0
5	C	37	Total 37	O 37	0	0
5	D	40	Total 40	O 40	0	0

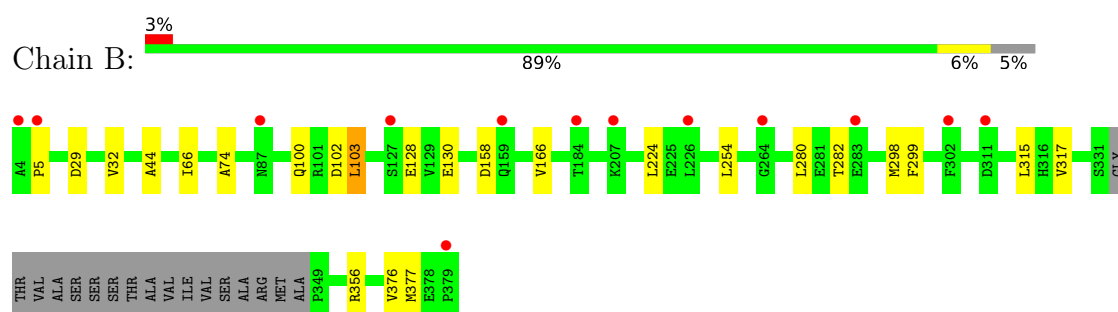
3 Residue-property plots [i](#)

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.

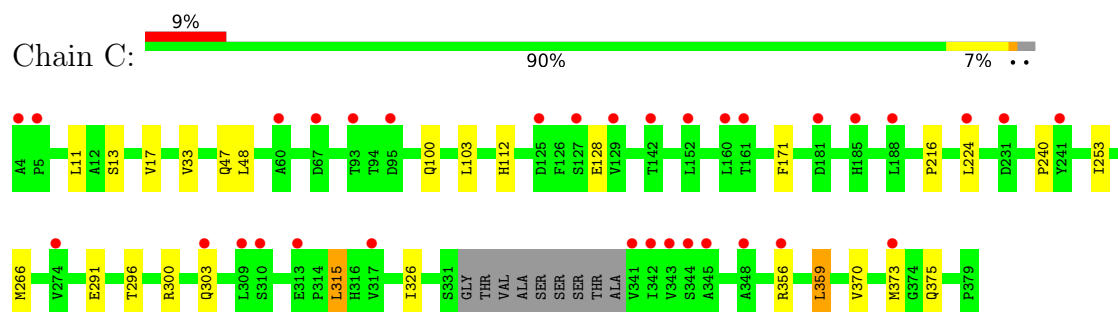
- Molecule 1: Plasminogen activator inhibitor 1



- Molecule 1: Plasminogen activator inhibitor 1

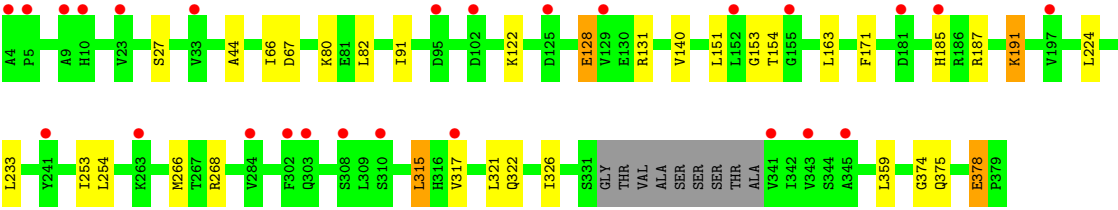


- Molecule 1: Plasminogen activator inhibitor 1



- Molecule 1: Plasminogen activator inhibitor 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.33Å 75.32Å 105.00Å 91.32° 93.49° 115.65°	Depositor
Resolution (Å)	20.00 – 2.71 20.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	87.6 (20.00-2.71) 87.5 (20.00-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.71Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2, BUSTER 2.11.2	Depositor
R, R_{free}	0.239 , 0.268 0.253 , 0.288	Depositor DCC
R_{free} test set	2158 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.894	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.5	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	0.91	EDS
Total number of atoms	11723	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: 96P, EDO, 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	0.74	0/2911	1.18	4/3951 (0.1%)
1	B	0.74	0/2922	1.17	3/3964 (0.1%)
1	C	0.74	0/2983	1.17	2/4046 (0.0%)
1	D	0.75	0/2952	1.16	1/4009 (0.0%)
All	All	0.74	0/11768	1.17	10/15970 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	216	PRO	CA-C-N	5.36	127.99	120.28
1	C	216	PRO	C-N-CA	5.36	127.99	120.28
1	B	128	GLU	CA-C-N	5.15	127.51	120.77
1	B	128	GLU	C-N-CA	5.15	127.51	120.77
1	A	128	GLU	CA-C-N	5.12	127.48	120.77
1	A	128	GLU	C-N-CA	5.12	127.48	120.77
1	D	374	GLY	N-CA-C	5.07	117.99	110.63
1	A	300	ARG	CA-C-N	5.04	127.34	120.54
1	A	300	ARG	C-N-CA	5.04	127.34	120.54

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	2841	0	2805	8	0
1	B	2851	0	2826	9	0
1	C	2912	0	2902	11	0
1	D	2881	0	2825	13	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	4	0	6	0	0
4	D	41	0	14	1	0
5	A	40	0	0	0	0
5	B	46	0	0	0	0
5	C	37	0	0	0	0
5	D	40	0	0	0	0
All	All	11723	0	11378	40	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 (40) 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:370:VAL:HG11	1:C:373:MET:HE3	1.74	0.70
1:B:29:ASP:HA	1:B:377:MET:HE2	1.86	0.58
1:C:171:PHE:HB3	1:C:326:ILE:HD13	1.87	0.56
1:D:163:LEU:HD23	1:D:317:VAL:HG22	1.89	0.55
1:D:191:LYS:HD3	1:D:378:GLU:HG3	1.87	0.55
1:B:130:GLU:HG2	1:C:11:LEU:HD23	1.87	0.54
1:C:300:ARG:HB3	1:C:303:GLN:HB2	1.88	0.54
1:C:240:PRO:HD2	1:C:356:ARG:HE	1.73	0.53
1:B:44:ALA:HB1	1:B:66:ILE:HD13	1.91	0.51
1:D:268:ARG:HH12	4:D:403:96P:H14	1.75	0.51
1:A:44:ALA:HB1	1:A:66:ILE:HD13	1.95	0.49
1:D:140:VAL:HG21	1:D:151:LEU:HD11	1.95	0.48
1:C:359:LEU:HD12	1:C:375:GLN:HB3	1.94	0.48
1:A:91:ILE:HG23	1:A:171:PHE:HD1	1.78	0.47
1:C:103:LEU:HD21	1:C:315:LEU:HD11	1.95	0.47
1:A:32:VAL:HG23	1:A:282:THR:HG21	1.96	0.47
1:D:171:PHE:HB3	1:D:326:ILE:HD13	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD13	1:A:165:LEU:HD13	1.96	0.46
1:D:151:LEU:HB2	1:D:154:THR:HG23	1.97	0.46
1:B:298:MET:HE3	1:B:317:VAL:HG21	1.98	0.46
1:C:291:GLU:HG2	1:C:296:THR:HA	1.98	0.45
1:A:29:ASP:HA	1:A:377:MET:HE2	1.99	0.45
1:C:13:SER:O	1:C:17:VAL:HG23	2.17	0.45
1:B:100:GLN:HB3	1:B:103:LEU:HD13	1.99	0.45
1:D:163:LEU:HB2	1:D:315:LEU:HD21	1.99	0.44
1:A:101:ARG:HA	1:A:123:GLN:HB3	1.99	0.44
1:A:309:LEU:HD23	1:A:315:LEU:HD13	2.00	0.44
1:B:5:PRO:HA	1:B:74:ALA:HB1	2.00	0.43
1:B:280:LEU:HD11	1:B:376:VAL:HG22	2.00	0.43
1:D:91:ILE:HD11	1:D:233:LEU:HD11	1.99	0.43
1:D:185:HIS:CE1	1:D:187:ARG:HE	2.37	0.42
1:D:359:LEU:HD12	1:D:375:GLN:HB3	2.01	0.42
1:D:44:ALA:HB1	1:D:66:ILE:HD13	2.02	0.42
1:B:32:VAL:HG23	1:B:282:THR:HG21	2.02	0.42
1:D:128:GLU:HB3	1:D:131:ARG:HB3	2.02	0.42
1:D:153:GLY:HA3	1:D:321:LEU:HD21	2.03	0.41
1:C:48:LEU:HD21	1:C:112:HIS:HD2	1.86	0.41
1:C:100:GLN:HB3	1:C:103:LEU:HB2	2.03	0.41
1:B:298:MET:HE2	1:B:299:PHE:CZ	2.56	0.40
1:A:20:PHE:HA	1:A:23:VAL:HG22	2.02	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	355/376 (94%)	344 (97%)	11 (3%)	0	100	100
1	B	355/376 (94%)	344 (97%)	11 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	363/376 (96%)	350 (96%)	13 (4%)	0	100	100
1	D	363/376 (96%)	353 (97%)	10 (3%)	0	100	100
All	All	1436/1504 (96%)	1391 (97%)	45 (3%)	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	310/329 (94%)	298 (96%)	12 (4%)	28	56
1	B	311/329 (94%)	304 (98%)	7 (2%)	44	71
1	C	319/329 (97%)	311 (98%)	8 (2%)	42	69
1	D	310/329 (94%)	296 (96%)	14 (4%)	24	50
All	All	1250/1316 (95%)	1209 (97%)	41 (3%)	33	61

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	47	GLN
1	A	53	GLU
1	A	91	ILE
1	A	103	LEU
1	A	152	LEU
1	A	188	LEU
1	A	214	THR
1	A	224	LEU
1	A	231	ASP
1	A	253	ILE
1	A	359	LEU
1	B	103	LEU
1	B	158	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	166	VAL
1	B	224	LEU
1	B	254	LEU
1	B	315	LEU
1	B	356	ARG
1	C	33	VAL
1	C	47	GLN
1	C	128	GLU
1	C	224	LEU
1	C	253	ILE
1	C	266	MET
1	C	315	LEU
1	C	359	LEU
1	D	27	SER
1	D	67	ASP
1	D	80	LYS
1	D	82	LEU
1	D	122	LYS
1	D	128	GLU
1	D	191	LYS
1	D	224	LEU
1	D	253	ILE
1	D	254	LEU
1	D	266	MET
1	D	315	LEU
1	D	322	GLN
1	D	378	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	87	ASN
1	A	174	GLN
1	A	209	ASN
1	A	252	ASN
1	A	292	ASN
1	A	312	GLN
1	A	316	HIS
1	A	329	ASN
1	B	174	GLN
1	B	292	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	GLN
1	B	316	HIS
1	C	22	GLN
1	C	25	GLN
1	C	112	HIS
1	C	190	HIS
1	C	301	GLN
1	C	329	ASN
1	D	22	GLN
1	D	47	GLN
1	D	172	ASN
1	D	265	ASN
1	D	292	ASN
1	D	316	HIS
1	D	329	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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	C	402	-	4,4,4	0.29	0	6,6,6	0.09	0
2	SO4	C	401	-	4,4,4	0.30	0	6,6,6	0.07	0
3	EDO	A	402	-	3,3,3	0.52	0	2,2,2	0.42	0
2	SO4	B	401	-	4,4,4	0.30	0	6,6,6	0.14	0
4	96P	D	403	-	43,43,43	0.26	0	60,62,62	0.81	1 (1%)
2	SO4	D	401	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	D	402	-	4,4,4	0.25	0	6,6,6	0.10	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	96P	D	403	-	-	5/32/32/32	0/3/3/3
3	EDO	A	402	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	96P	O7-C3-C2	5.32	116.41	107.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

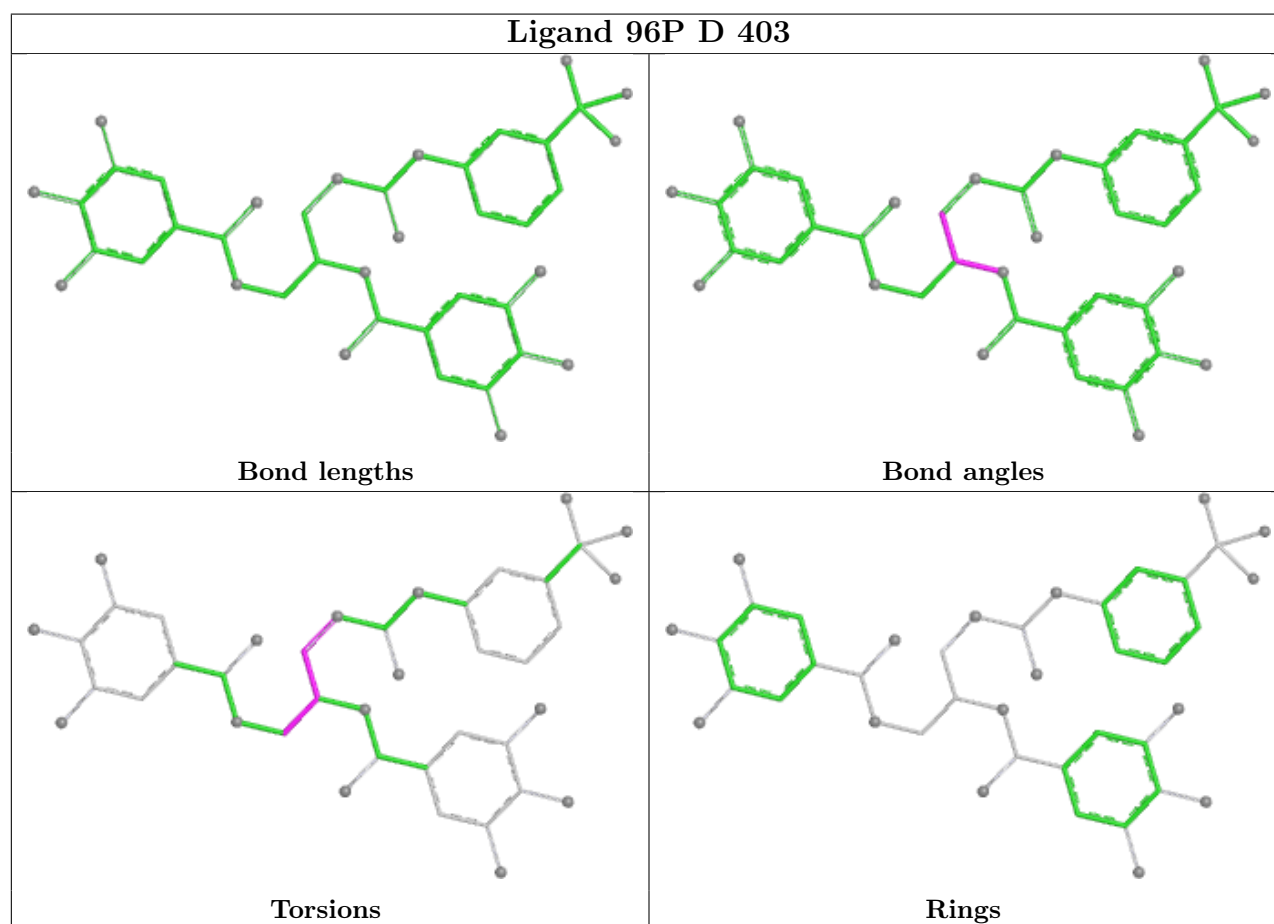
Mol	Chain	Res	Type	Atoms
4	D	403	96P	N-C2-C3-O7
4	D	403	96P	N-C2-C3-C4
4	D	403	96P	C2-C3-C4-O2
4	D	403	96P	O7-C3-C4-O2
4	D	403	96P	C3-C2-N-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	96P	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	359/376 (95%)	0.84	21 (5%) 29 26	37, 53, 65, 69	0
1	B	359/376 (95%)	0.77	13 (3%) 46 43	38, 53, 66, 73	0
1	C	367/376 (97%)	0.95	33 (8%) 15 13	38, 57, 86, 125	0
1	D	367/376 (97%)	0.85	26 (7%) 22 19	40, 57, 66, 73	0
All	All	1452/1504 (96%)	0.85	93 (6%) 25 23	37, 55, 72, 125	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	VAL	5.5
1	A	5	PRO	4.9
1	C	5	PRO	4.6
1	B	4	ALA	4.3
1	B	5	PRO	4.3
1	D	5	PRO	4.3
1	C	342	ILE	4.2
1	A	4	ALA	4.1
1	C	343	VAL	4.0
1	C	4	ALA	3.8
1	C	345	ALA	3.6
1	C	356	ARG	3.6
1	A	102	ASP	3.5
1	D	125	ASP	3.5
1	C	125	ASP	3.4
1	D	10	HIS	3.3
1	C	348	ALA	3.2
1	D	241	TYR	3.1
1	C	129	VAL	3.1
1	A	29	ASP	3.0
1	D	4	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	127	SER	2.9
1	D	95	ASP	2.9
1	B	264	GLY	2.9
1	A	128	GLU	2.9
1	D	129	VAL	2.9
1	D	185	HIS	2.9
1	B	311	ASP	2.8
1	D	102	ASP	2.8
1	B	184	THR	2.8
1	D	197	VAL	2.8
1	C	344	SER	2.8
1	B	87	ASN	2.7
1	C	231	ASP	2.7
1	D	155	GLY	2.6
1	C	241	TYR	2.6
1	C	373	MET	2.6
1	C	224	LEU	2.6
1	C	303	GLN	2.6
1	D	310	SER	2.6
1	C	185	HIS	2.6
1	A	313	GLU	2.6
1	B	302	PHE	2.5
1	A	307	THR	2.5
1	D	152	LEU	2.5
1	D	343	VAL	2.5
1	A	136	ILE	2.4
1	C	95	ASP	2.4
1	B	159	GLN	2.4
1	C	93	THR	2.4
1	A	297	ASP	2.4
1	D	181	ASP	2.4
1	C	188	LEU	2.3
1	D	263	LYS	2.3
1	A	95	ASP	2.3
1	C	161	THR	2.2
1	C	67	ASP	2.2
1	A	146	GLY	2.2
1	C	317	VAL	2.2
1	B	226	LEU	2.2
1	C	60	ALA	2.2
1	C	181	ASP	2.2
1	D	303	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	6	SER	2.2
1	D	284	VAL	2.2
1	D	317	VAL	2.2
1	D	341	VAL	2.2
1	C	152	LEU	2.1
1	C	309	LEU	2.1
1	A	157	VAL	2.1
1	A	311	ASP	2.1
1	B	127	SER	2.1
1	C	274	VAL	2.1
1	A	208	PHE	2.1
1	B	379	PRO	2.1
1	C	127	SER	2.1
1	D	308	SER	2.1
1	A	203	ALA	2.1
1	D	345	ALA	2.1
1	B	283	GLU	2.1
1	D	23	VAL	2.1
1	A	302	PHE	2.1
1	C	310	SER	2.1
1	B	207	LYS	2.1
1	D	302	PHE	2.1
1	C	313	GLU	2.0
1	D	9	ALA	2.0
1	C	142	THR	2.0
1	A	349	PRO	2.0
1	C	160	LEU	2.0
1	A	173	GLY	2.0
1	A	287	ARG	2.0
1	D	33	VAL	2.0

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 ⓘ

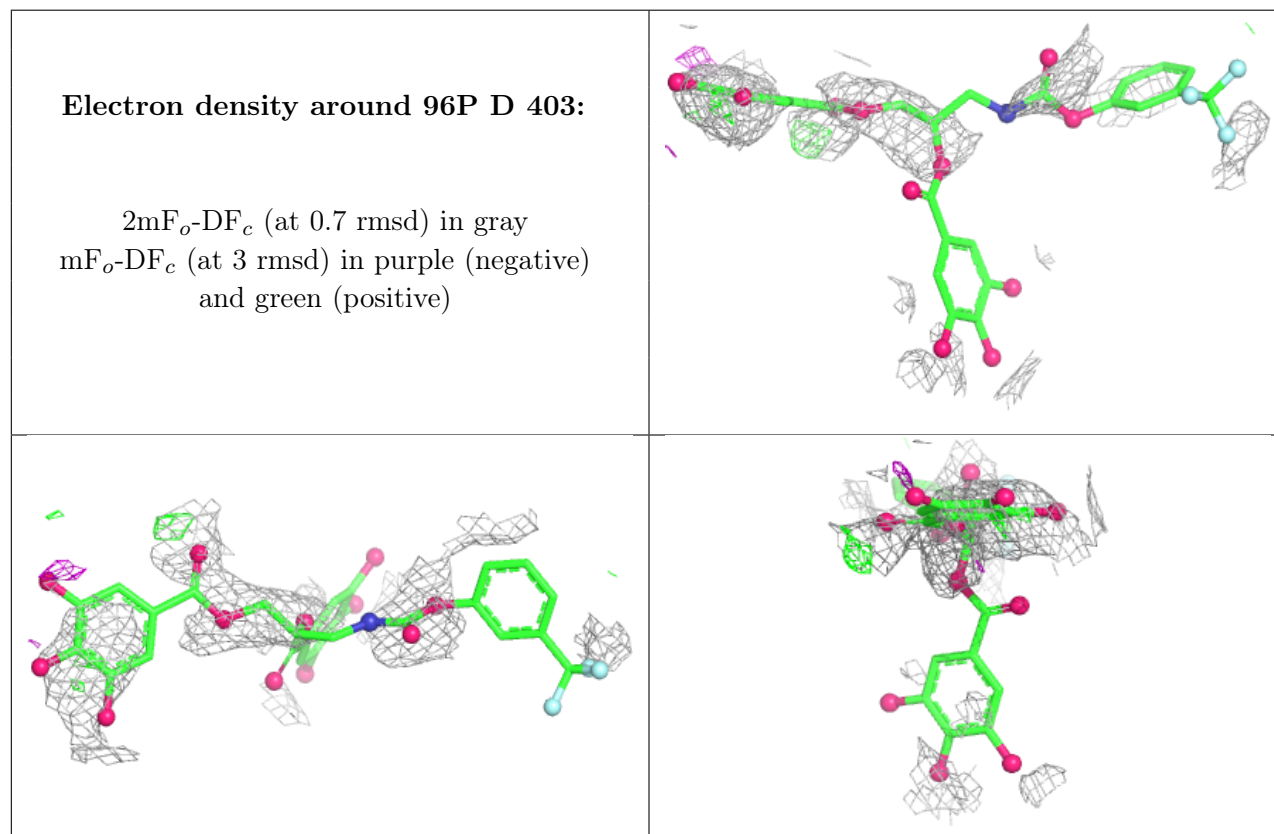
There are no oligosaccharides in this entry.

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
4	96P	D	403	41/41	0.68	0.28	85,85,85,85	41
3	EDO	A	402	4/4	0.76	0.14	40,40,40,40	0
2	SO4	B	401	5/5	0.88	0.10	68,68,68,69	0
2	SO4	D	401	5/5	0.88	0.08	86,86,87,87	0
2	SO4	C	402	5/5	0.89	0.12	81,81,81,81	0
2	SO4	C	401	5/5	0.91	0.09	69,70,70,70	0
2	SO4	A	401	5/5	0.92	0.07	67,67,67,67	0
2	SO4	D	402	5/5	0.92	0.11	77,78,78,78	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 [i](#)

There are no such residues in this entry.