WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 06:38 PM EST

PDB ID	:	4G8O
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)

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

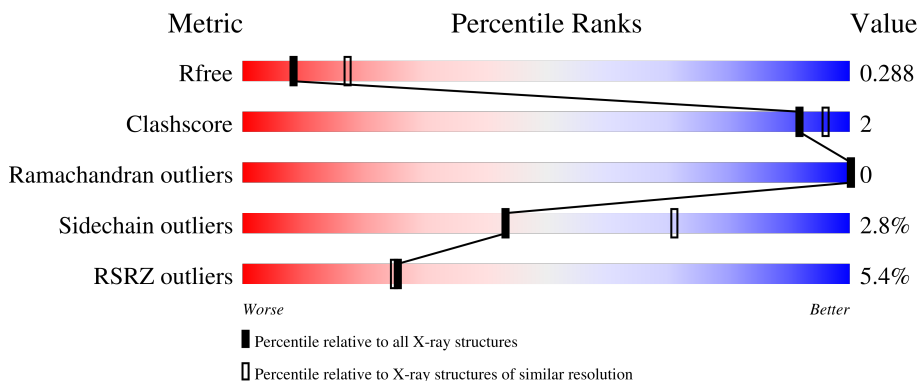|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.288
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		2.8%
RSRZ outliers		5.4%

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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (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 <=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	5%; 89%; 6%; 5%
1	B	376	3%; 91%; •; 5%
1	C	376	6%; 91%; 6%; •
1	D	376	7%; 89%; 8%; ••

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
4	96P	D	403	-	-	-	X

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 (three-letter code: SO4) (formula: O_4S).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

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

- Molecule 4 is (2S)-3-({[3-(trifluoromethyl)phenoxy]carbonyl}amino)propane-1,2-diyl bis(3,4 ,5-trihydroxybenzoate) (three-letter code: 96P) (formula: $C_{25}H_{20}F_3NO_{12}$).

96P
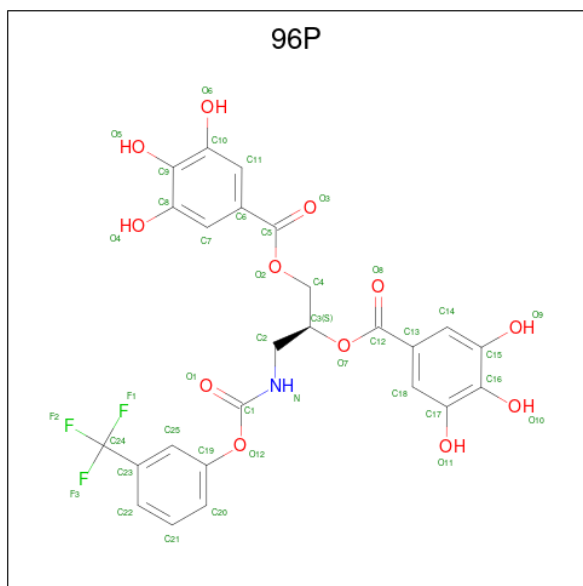
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 41	C 25	F 3	N 1	O 12	21	0

- Molecule 5 is water.

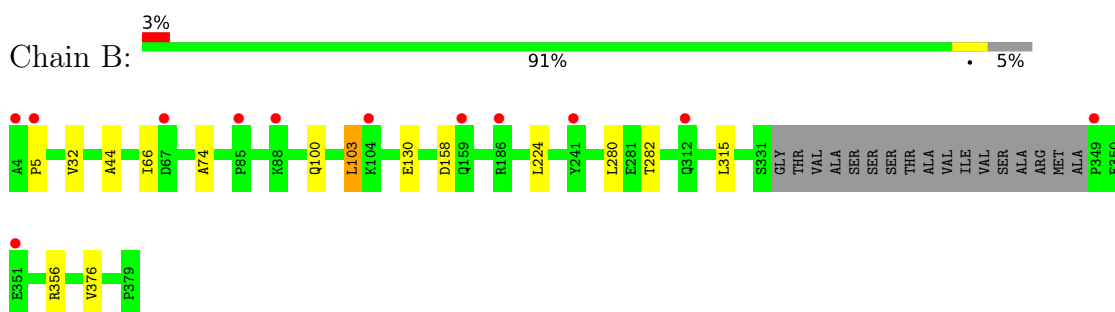| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	40	Total O 40 40	0	0
5	B	46	Total O 46 46	0	0
5	C	37	Total O 37 37	0	0
5	D	40	Total O 40 40	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Plasminogen activator inhibitor 1
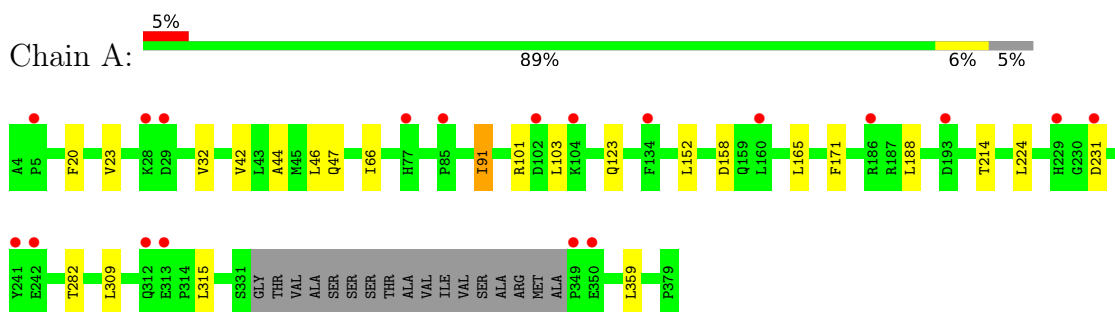
Chain A:

• Molecule 1: Plasminogen activator inhibitor 1

Chain B:

• Molecule 1: Plasminogen activator inhibitor 1

Chain C:

• Molecule 1: Plasminogen activator inhibitor 1

Chain D:

A4 P5 S6 S27 K28 D29 R30 A44 E53 Q56 I66 D67 K80 E81 L82 I91 D102 K122 D125 F126 S127 E128 V129 E130 R131 V140 L151 L152 G153 T154 G155 Q159 L163 F171 D181 S182 H185 R186 R187 K191 S192 D193

T196 V197 L224 L233 Y241 E244 L254 R268 L269 P270 F302 S310 D311 P314 L315 H316 V317 L321 Q322 I326 S331 GLY THR VAL ALA SER SER THR ALA V341 E351 L359 Q375 E378 P379
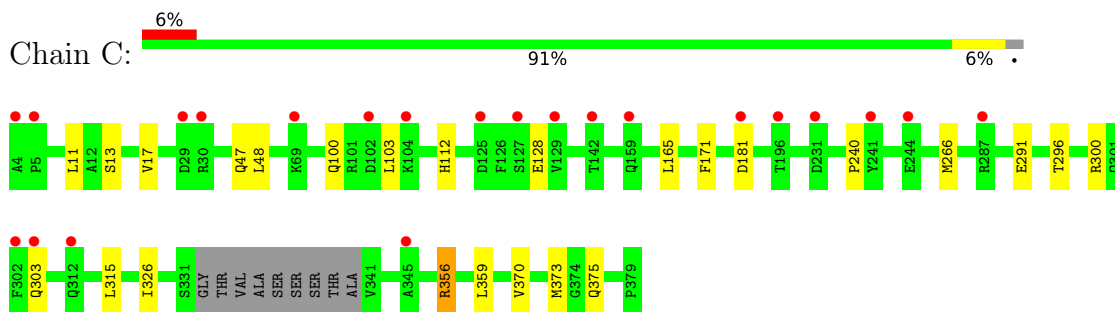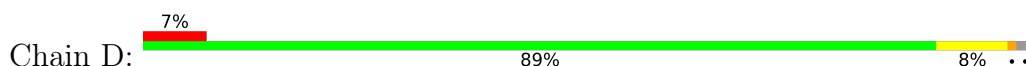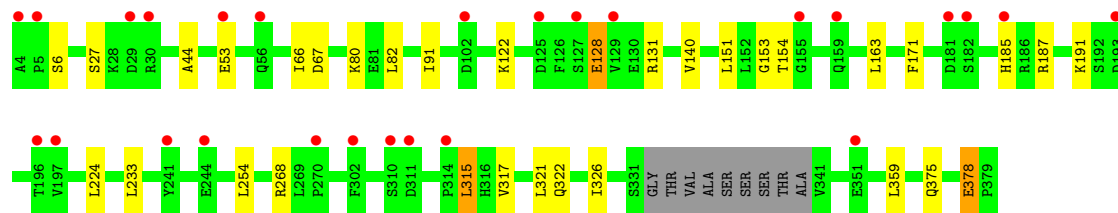
4 Data and refinement statistics (i)

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 20.32 – 2.71	Depositor EDS
% Data completeness (in resolution range)	87.6 (20.00-2.71) 87.7 (20.32-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.33 , 51.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

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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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, 96P

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	0.39	0/2911	0.57	0/3951
1	B	0.39	0/2922	0.56	0/3964
1	C	0.39	0/2983	0.55	0/4046
1	D	0.40	0/2952	0.56	0/4009
All	All	0.39	0/11768	0.56	0/15970

There are no bond length outliers.

There are no bond angle outliers.

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	7	0
1	B	2851	0	2826	6	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	36	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 (36) 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: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:C:370:VAL:HG11	1:C:373:MET:HE3	1.97	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
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:C:291:GLU:HG2	1:C:296:THR:HA	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:20:PHE:HA	1:A:23:VAL:HG22	2.02	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	355/376 (94%)	344 (97%)	11 (3%)	0	100	100
1	B	355/376 (94%)	344 (97%)	11 (3%)	0	100	100
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%)	299 (96%)	11 (4%)	36	63
1	B	311/329 (94%)	306 (98%)	5 (2%)	62	83
1	C	319/329 (97%)	313 (98%)	6 (2%)	57	81
1	D	310/329 (94%)	297 (96%)	13 (4%)	30	56
All	All	1250/1316 (95%)	1215 (97%)	35 (3%)	43	71

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	47	GLN
1	A	91	ILE
1	A	103	LEU
1	A	152	LEU
1	A	158	ASP
1	A	188	LEU
1	A	214	THR
1	A	224	LEU
1	A	231	ASP
1	A	359	LEU
1	B	103	LEU
1	B	158	ASP
1	B	224	LEU
1	B	315	LEU
1	B	356	ARG
1	C	47	GLN
1	C	128	GLU
1	C	165	LEU
1	C	181	ASP
1	C	266	MET
1	C	356	ARG
1	D	6	SER
1	D	27	SER
1	D	53	GLU
1	D	67	ASP
1	D	80	LYS
1	D	82	LEU
1	D	122	LYS
1	D	128	GLU
1	D	224	LEU
1	D	254	LEU
1	D	315	LEU

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Mol	Chain	Res	Type
1	D	322	GLN
1	D	378	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	HIS
1	C	112	HIS
1	C	190	HIS
1	D	59	GLN

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 ⓘ

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	D	402	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	C	401	-	4,4,4	0.20	0	6,6,6	0.06	0
2	SO4	D	401	-	4,4,4	0.13	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	C	402	-	4,4,4	0.17	0	6,6,6	0.06	0
3	EDO	A	402	-	3,3,3	0.58	0	2,2,2	0.37	0
2	SO4	A	401	-	4,4,4	0.12	0	6,6,6	0.04	0
4	96P	D	403	-	43,43,43	0.27	0	59,62,62	0.44	0
2	SO4	B	401	-	4,4,4	0.20	0	6,6,6	0.11	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.

There are no bond angle outliers.

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	C3-C2-N-C1
4	D	403	96P	O7-C3-C4-O2

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 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 96P D 403

Bond lengths

Bond angles

Torsions

Rings
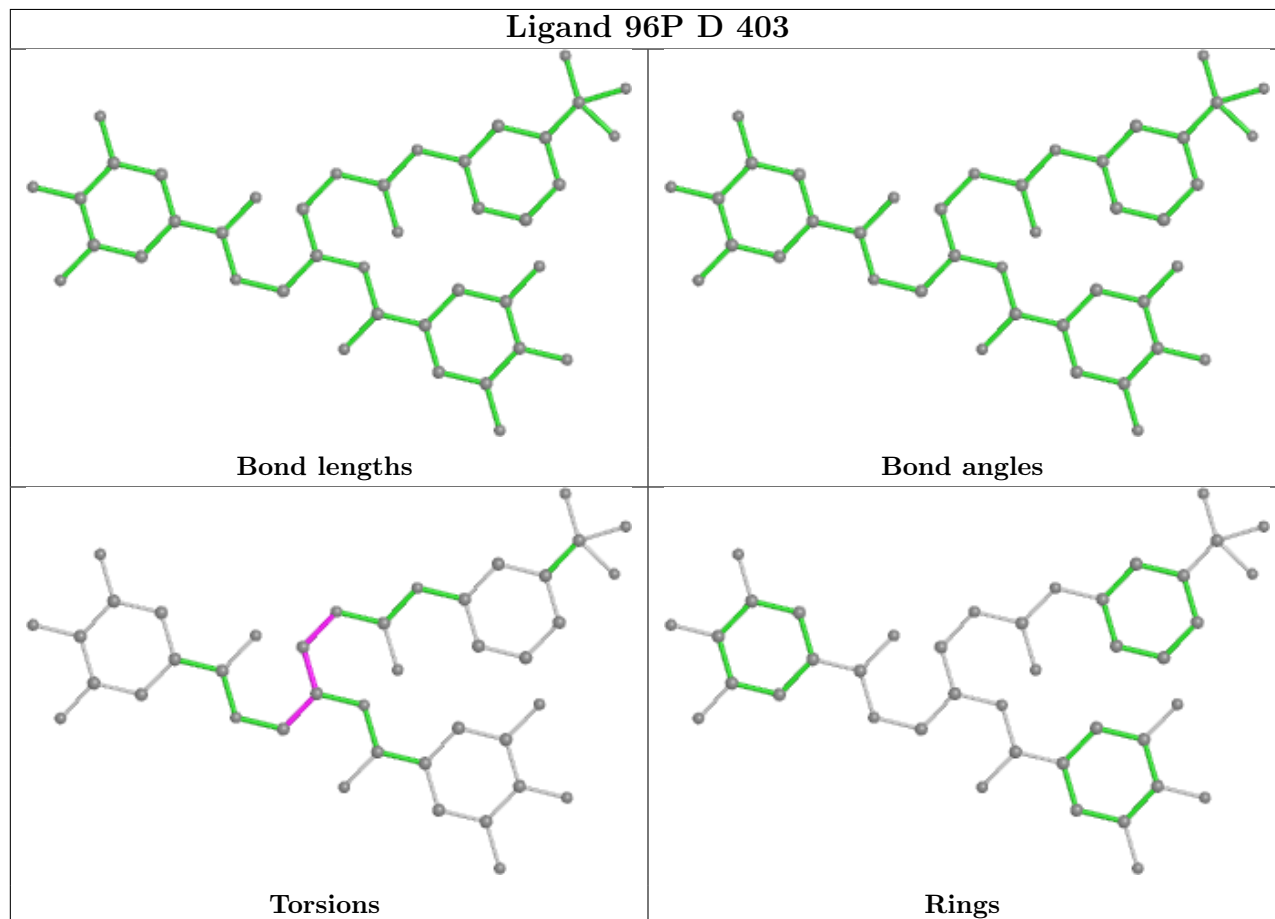
5.7 Other polymers ⓘ

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	359/376 (95%)	0.33	19 (5%)	26	25	37, 53, 65, 69	0
1	B	359/376 (95%)	0.30	12 (3%)	46	47	38, 53, 66, 73	0
1	C	367/376 (97%)	0.50	22 (5%)	21	21	38, 57, 86, 125	0
1	D	367/376 (97%)	0.46	26 (7%)	16	14	40, 57, 66, 73	0
All	All	1452/1504 (96%)	0.40	79 (5%)	25	25	37, 55, 72, 125	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	PRO	6.9
1	D	5	PRO	5.0
1	A	102	ASP	4.5
1	D	125	ASP	4.5
1	D	302	PHE	4.3
1	C	196	THR	4.2
1	C	4	ALA	4.2
1	D	241	TYR	4.0
1	C	181	ASP	3.9
1	D	181	ASP	3.8
1	C	159	GLN	3.8
1	D	197	VAL	3.7
1	C	303	GLN	3.7
1	C	241	TYR	3.7
1	B	4	ALA	3.6
1	B	85	PRO	3.6
1	C	125	ASP	3.6
1	A	5	PRO	3.4
1	D	310	SER	3.4
1	C	104	LYS	3.4
1	D	4	ALA	3.3

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type	RSRZ
1	D	102	ASP	3.2
1	D	196	THR	3.0
1	C	231	ASP	2.9
1	C	244	GLU	2.9
1	A	312	GLN	2.9
1	D	53	GLU	2.9
1	B	241	TYR	2.8
1	A	241	TYR	2.7
1	B	312	GLN	2.6
1	B	186	ARG	2.5
1	D	244	GLU	2.5
1	A	134	PHE	2.5
1	A	231	ASP	2.5
1	D	314	PRO	2.5
1	C	127	SER	2.5
1	D	182	SER	2.5
1	D	129	VAL	2.5
1	D	351	GLU	2.4
1	C	345	ALA	2.4
1	A	186	ARG	2.4
1	B	104	LYS	2.4
1	C	312	GLN	2.4
1	C	29	ASP	2.3
1	C	102	ASP	2.3
1	A	160	LEU	2.3
1	B	88	LYS	2.3
1	A	350	GLU	2.3
1	D	127	SER	2.3
1	A	313	GLU	2.3
1	D	155	GLY	2.3
1	B	5	PRO	2.2
1	A	242	GLU	2.2
1	C	302	PHE	2.2
1	C	69	LYS	2.2
1	A	349	PRO	2.2
1	B	349	PRO	2.2
1	D	270	PRO	2.2
1	B	67	ASP	2.2
1	A	104	LYS	2.2
1	C	287	ARG	2.2
1	A	229	HIS	2.2
1	A	28	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	85	PRO	2.2
1	C	142	THR	2.1
1	D	159	GLN	2.1
1	A	29	ASP	2.1
1	D	193	ASP	2.1
1	D	56	GLN	2.1
1	D	185	HIS	2.1
1	D	311	ASP	2.1
1	B	351	GLU	2.1
1	A	77	HIS	2.1
1	B	159	GLN	2.1
1	C	129	VAL	2.1
1	A	193	ASP	2.0
1	D	29	ASP	2.0
1	C	30	ARG	2.0
1	D	30	ARG	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 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.
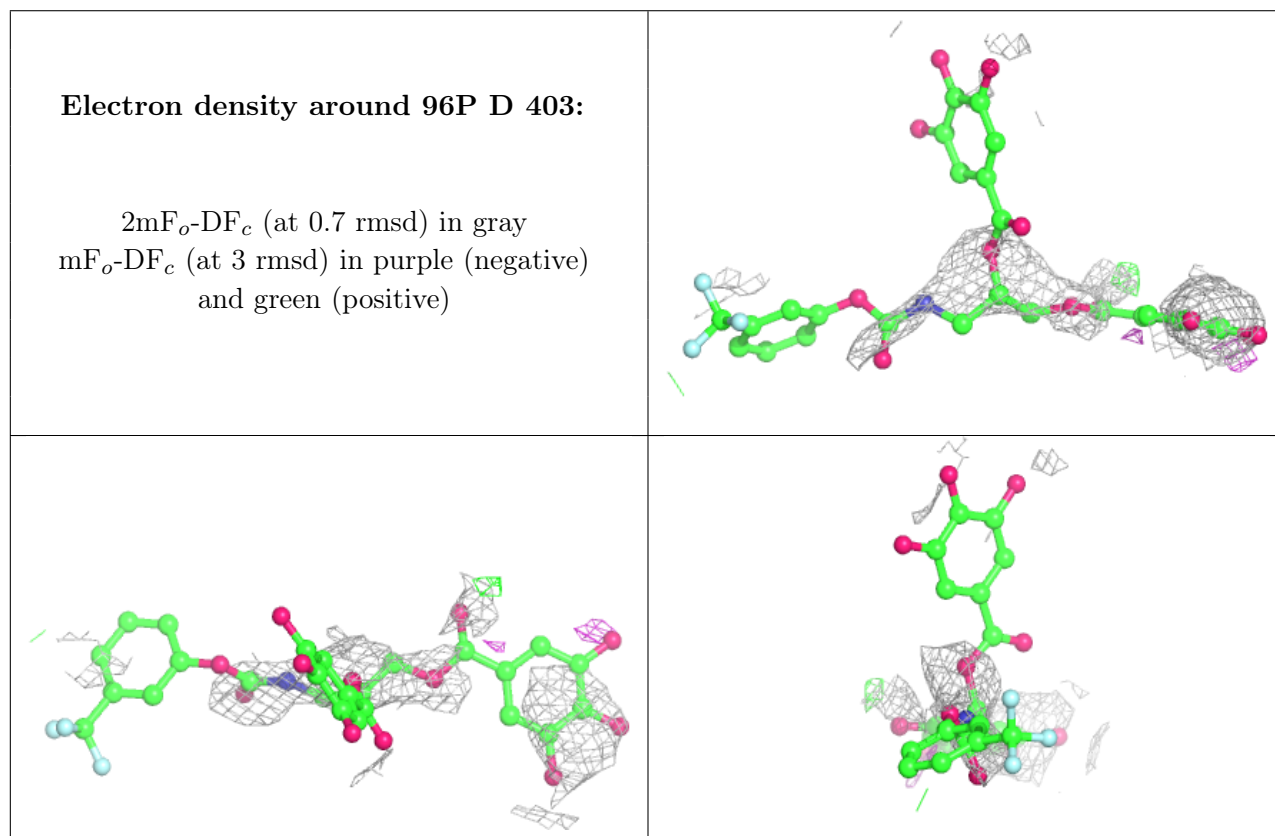
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	96P	D	403	41/41	0.68	0.47	85,85,85,85	41
3	EDO	A	402	4/4	0.91	0.16	40,40,40,40	0
2	SO4	D	401	5/5	0.93	0.15	86,86,87,87	0
2	SO4	C	402	5/5	0.95	0.12	81,81,81,81	0
2	SO4	D	402	5/5	0.95	0.20	77,78,78,78	0
2	SO4	C	401	5/5	0.96	0.10	69,70,70,70	0
2	SO4	B	401	5/5	0.96	0.12	68,68,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	401	5/5	0.98	0.08	67,67,67,67	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 96P D 403:

$2mF_o\text{-}DF_c$ (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.