



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:34 AM UTC

PDB ID : 9GOD / pdb\_00009god  
Title : Crystal structure of DPP9 in complex with N-phosphono-(S)-3-aminopiperidine-2-one-based inhibitor  
Authors : Sewald, L.; Tabak, W.W.A.; Fehr, L.; Zolg, S.; Najdzion, M.; Verhoef, C.J.A.; Podlesainski, D.; Geiss-Friedlander, R.; Lammens, A.; Kaschani, F.; Hellerschmied, D.; Huber, R.; Kaiser, M.  
Deposited on : 2024-09-05  
Resolution : 2.49 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) 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

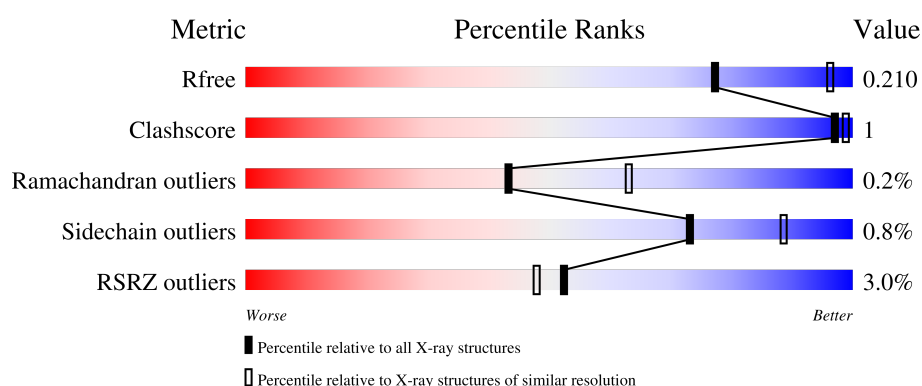
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	851	<div> <div>2%</div> <div>93%</div> <div>5%</div> <div>• •</div> </div>
1	B	851	<div> <div>0%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>
1	C	851	<div> <div>0%</div> <div>92%</div> <div>5%</div> <div>• •</div> </div>
1	D	851	<div> <div>7%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27151 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 Dipeptidyl peptidase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	816	Total	C	N	O	S	70	3	0
			6609	4246	1122	1211	30			
1	B	815	Total	C	N	O	S	80	2	0
			6597	4237	1122	1209	29			
1	C	816	Total	C	N	O	S	59	6	0
			6642	4264	1131	1216	31			
1	D	798	Total	C	N	O	S	240	0	0
			6449	4150	1093	1177	29			

There are 28 discrepancies between the modelled and reference sequences:

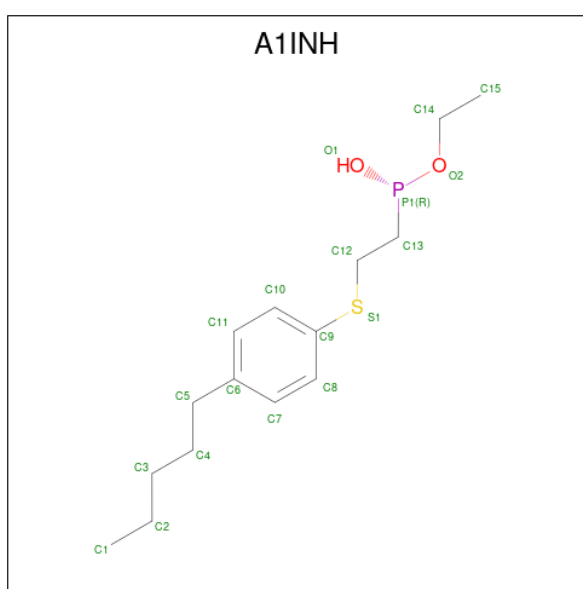
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP Q86TI2
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	19	MET	-	initiating methionine	UNP Q86TI2
B	864	HIS	-	expression tag	UNP Q86TI2
B	865	HIS	-	expression tag	UNP Q86TI2
B	866	HIS	-	expression tag	UNP Q86TI2
B	867	HIS	-	expression tag	UNP Q86TI2
B	868	HIS	-	expression tag	UNP Q86TI2
B	869	HIS	-	expression tag	UNP Q86TI2
C	19	MET	-	initiating methionine	UNP Q86TI2
C	864	HIS	-	expression tag	UNP Q86TI2
C	865	HIS	-	expression tag	UNP Q86TI2
C	866	HIS	-	expression tag	UNP Q86TI2
C	867	HIS	-	expression tag	UNP Q86TI2
C	868	HIS	-	expression tag	UNP Q86TI2
C	869	HIS	-	expression tag	UNP Q86TI2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	MET	-	initiating methionine	UNP Q86TI2
D	864	HIS	-	expression tag	UNP Q86TI2
D	865	HIS	-	expression tag	UNP Q86TI2
D	866	HIS	-	expression tag	UNP Q86TI2
D	867	HIS	-	expression tag	UNP Q86TI2
D	868	HIS	-	expression tag	UNP Q86TI2
D	869	HIS	-	expression tag	UNP Q86TI2

- Molecule 2 is ethoxy-[2-(4-pentylphenyl)sulfanylethyl]phosphinous acid (CCD ID: A1INH) (formula: C<sub>15</sub>H<sub>25</sub>O<sub>2</sub>PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	O	P	S	0	0
			19	15	2	1	1		
2	B	1	Total	C	O	P	S	4	0
			19	15	2	1	1		
2	C	1	Total	C	O	P	S	3	0
			19	15	2	1	1		
2	D	1	Total	C	O	P	S	3	0
			19	15	2	1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

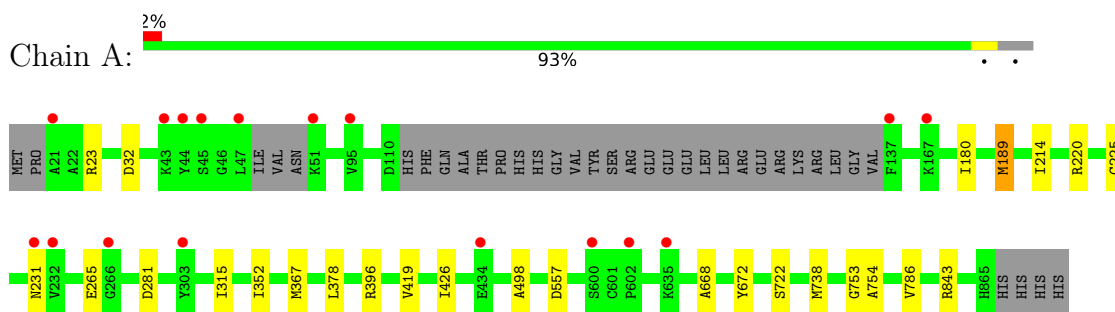
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total 136	O 136	0	0
5	B	216	Total 216	O 216	0	1
5	C	242	Total 242	O 242	0	0
5	D	42	Total 42	O 42	0	0

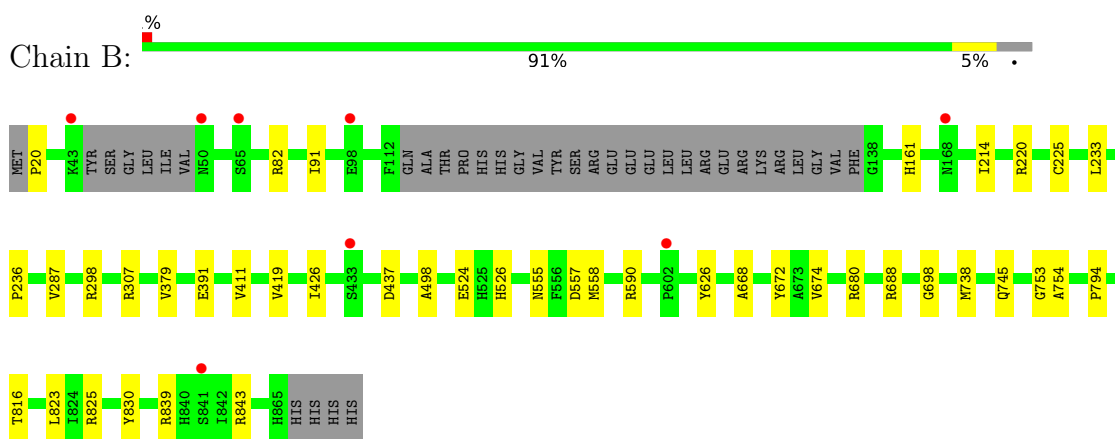
### 3 Residue-property plots [i](#)

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.

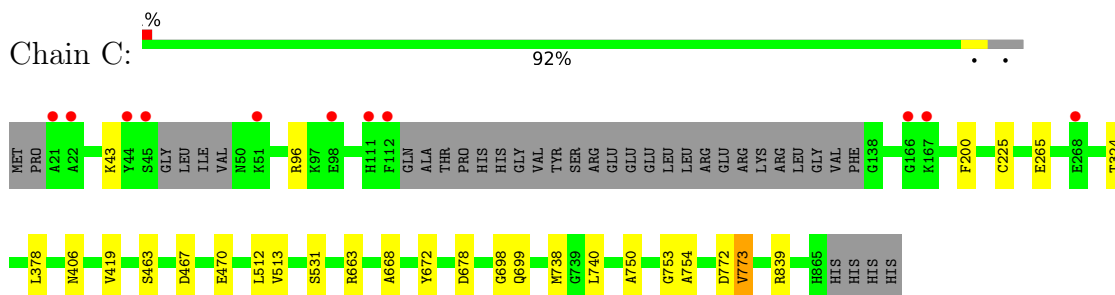
- Molecule 1: Dipeptidyl peptidase 9



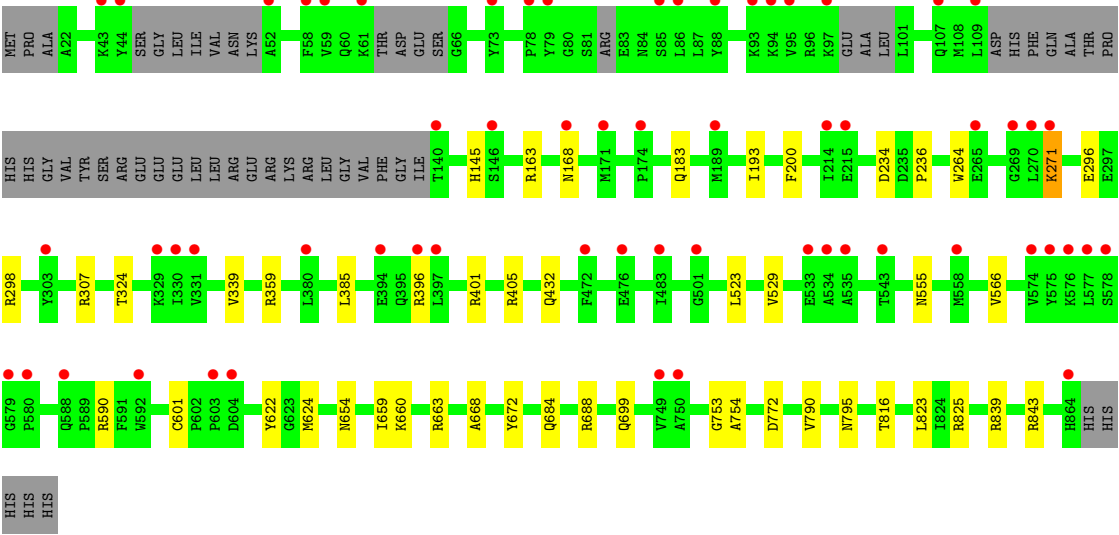
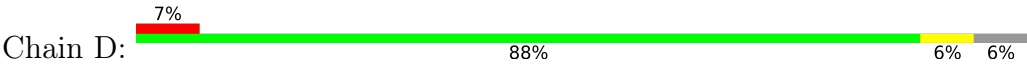
- Molecule 1: Dipeptidyl peptidase 9



- Molecule 1: Dipeptidyl peptidase 9



- Molecule 1: Dipeptidyl peptidase 9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.31Å 106.75Å 121.48Å 65.24° 71.02° 76.71°	Depositor
Resolution (Å)	106.55 – 2.49 106.55 – 2.49	Depositor EDS
% Data completeness (in resolution range)	72.3 (106.55-2.49) 72.5 (106.55-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.170 , 0.219 (Not available) , 0.210	Depositor DCC
$R_{free}$ test set	238 reflections (0.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27151	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1INH, EDO, CL

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	0.57	1/6808 (0.0%)	0.95	3/9240 (0.0%)
1	B	0.58	4/6797 (0.1%)	0.97	4/9226 (0.0%)
1	C	0.57	1/6842 (0.0%)	0.96	6/9285 (0.1%)
1	D	0.62	7/6643 (0.1%)	0.98	7/9014 (0.1%)
All	All	0.58	13/27090 (0.0%)	0.97	20/36765 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	1
1	D	0	4
All	All	0	9

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	688	ARG	NE-CZ	10.52	1.44	1.33
1	D	405	ARG	NE-CZ	10.11	1.44	1.33
1	D	590	ARG	NE-CZ	9.41	1.43	1.33
1	D	843	ARG	NE-CZ	9.32	1.43	1.33
1	A	843	ARG	NE-CZ	8.23	1.42	1.33
1	C	96	ARG	NE-CZ	7.83	1.41	1.33
1	D	401	ARG	NE-CZ	7.59	1.41	1.33
1	D	825	ARG	NE-CZ	7.55	1.41	1.33
1	B	688	ARG	NE-CZ	6.77	1.40	1.33
1	B	843	ARG	NE-CZ	6.75	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	ARG	NE-CZ	5.34	1.39	1.33
1	D	359	ARG	NE-CZ	5.13	1.38	1.33
1	B	590	ARG	NE-CZ	5.12	1.38	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	236	PRO	N-CA-C	8.49	124.47	114.03
1	B	437	ASP	CA-CB-CG	6.44	119.04	112.60
1	D	699	GLN	CB-CA-C	6.44	121.48	110.86
1	B	236	PRO	N-CD-CG	-6.43	93.56	103.20
1	C	225	CYS	CB-CA-C	-6.42	99.93	110.85
1	D	396	ARG	CD-NE-CZ	6.33	133.27	124.40
1	D	234	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	557	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	281	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	772	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	271	LYS	N-CA-CB	5.55	118.19	109.69
1	C	699	GLN	CB-CA-C	5.50	119.93	110.86
1	C	773	VAL	N-CA-CB	-5.40	103.65	111.21
1	A	225	CYS	CB-CA-C	-5.39	100.84	110.70
1	C	678	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	467	ASP	CA-CB-CG	5.08	117.67	112.60
1	B	225	CYS	CB-CA-C	-5.04	101.48	110.70
1	B	557	ASP	CA-CB-CG	5.02	117.62	112.60
1	C	772	ASP	CA-CB-CG	5.01	117.61	112.60
1	D	432	GLN	CB-CA-C	5.00	119.62	112.12

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	ARG	Sidechain
1	B	298	ARG	Sidechain
1	B	307	ARG	Sidechain
1	B	680	ARG	Sidechain
1	C	663	ARG	Sidechain
1	D	163	ARG	Sidechain
1	D	298	ARG	Sidechain
1	D	307	ARG	Sidechain
1	D	663	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6609	0	6382	11	0
1	B	6597	0	6367	14	0
1	C	6642	0	6410	7	0
1	D	6449	0	6233	13	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	0	0
2	D	19	0	0	0	0
3	A	36	0	54	0	0
3	B	48	0	72	0	0
3	C	44	0	66	0	0
3	D	12	0	18	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	136	0	0	0	0
5	B	216	0	0	2	0
5	C	242	0	0	0	0
5	D	42	0	0	0	0
All	All	27151	0	25602	44	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 1.

All (44) 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:D:264:TRP:CZ3	1:D:271:LYS:HG2	2.41	0.56
1:A:180:ILE:HD11	1:A:214:ILE:HD11	1.91	0.53
1:A:231[B]:ASN:OD1	1:A:231[B]:ASN:N	2.38	0.51
1:B:825:ARG:NH1	5:B:1007:HOH:O	2.43	0.51
1:A:738:MET:HE2	1:A:786:VAL:HG12	1.93	0.51
1:D:200:PHE:CZ	1:D:324:THR:HG21	2.46	0.51
1:A:367:MET:HE2	1:A:378:LEU:HD21	1.93	0.50
1:D:339:VAL:HG23	1:D:385:LEU:O	2.11	0.50
1:A:668:ALA:HA	1:A:672:TYR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:MET:HE1	3:D:904:EDO:O1	2.12	0.49
1:B:626:TYR:HB2	1:B:674:VAL:HB	1.95	0.48
1:B:698:GLY:HA3	1:B:738:MET:HE2	1.97	0.47
1:B:91:ILE:HG21	1:B:558:MET:SD	2.55	0.47
1:B:524:GLU:OE1	1:B:526:HIS:HE1	1.98	0.46
1:D:668:ALA:HA	1:D:672:TYR:O	2.15	0.46
1:C:512:LEU:HD23	1:C:531:SER:HA	1.98	0.45
1:B:668:ALA:HA	1:B:672:TYR:O	2.16	0.45
1:B:823:LEU:HD13	1:B:830:TYR:HB3	1.99	0.45
1:C:406:ASN:HA	1:C:463:SER:OG	2.17	0.44
1:A:426:ILE:HD12	1:A:498:ALA:HB2	1.98	0.44
1:D:659:ILE:HG13	1:D:660:LYS:N	2.32	0.44
1:A:32:ASP:OD2	1:D:795:ASN:ND2	2.50	0.44
1:B:379:VAL:HG22	1:B:411:VAL:HG22	2.01	0.43
1:B:745[A]:GLN:H	1:B:745[A]:GLN:CD	2.24	0.43
1:D:145:HIS:HB2	1:D:193:ILE:HD13	2.01	0.43
1:B:753:GLY:O	1:B:754:ALA:C	2.62	0.42
1:D:790:VAL:HG13	1:D:823:LEU:HD23	2.01	0.42
1:A:189:MET:HA	1:A:189:MET:HE2	2.00	0.42
1:A:315:ILE:HD12	1:A:352:ILE:HG13	2.02	0.42
1:D:523:LEU:HD21	1:D:622:TYR:CD2	2.53	0.42
1:B:233:LEU:HD11	1:B:287:VAL:HG21	2.00	0.42
1:D:753:GLY:O	1:D:754:ALA:C	2.62	0.42
1:B:161:HIS:CG	1:B:214:ILE:HD11	2.54	0.42
1:A:23:ARG:NH1	1:A:722:SER:OG	2.53	0.42
1:C:668:ALA:HA	1:C:672:TYR:O	2.19	0.41
1:C:753:GLY:O	1:C:754:ALA:C	2.63	0.41
1:B:794:PRO:HA	5:B:1069:HOH:O	2.20	0.41
1:C:200:PHE:CZ	1:C:324:THR:HG21	2.55	0.41
1:A:753:GLY:O	1:A:754:ALA:C	2.63	0.41
1:D:566:VAL:HG13	1:D:654:ASN:HA	2.01	0.41
1:B:426:ILE:HD12	1:B:498:ALA:HB2	2.03	0.40
1:D:145:HIS:HB2	1:D:193:ILE:CD1	2.51	0.40
1:C:698:GLY:HA3	1:C:738:MET:HE2	2.03	0.40
1:C:740:LEU:HD22	1:C:750:ALA:HB3	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	813/851 (96%)	783 (96%)	29 (4%)	1 (0%)	48	68
1	B	811/851 (95%)	782 (96%)	27 (3%)	2 (0%)	43	63
1	C	816/851 (96%)	790 (97%)	24 (3%)	2 (0%)	43	63
1	D	786/851 (92%)	758 (96%)	27 (3%)	1 (0%)	48	68
All	All	3226/3404 (95%)	3113 (96%)	107 (3%)	6 (0%)	43	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	839	ARG
1	D	839	ARG
1	C	839	ARG
1	A	419	VAL
1	B	419	VAL
1	C	419	VAL

### 5.3.2 Protein sidechains [i](#)

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	719/748 (96%)	716 (100%)	3 (0%)	84	93
1	B	718/748 (96%)	713 (99%)	5 (1%)	76	89
1	C	723/748 (97%)	717 (99%)	6 (1%)	73	88
1	D	702/748 (94%)	694 (99%)	8 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2862/2992 (96%)	2840 (99%)	22 (1%)	73 88

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	MET
1	A	220	ARG
1	A	265	GLU
1	B	20	PRO
1	B	220	ARG
1	B	391	GLU
1	B	555	ASN
1	B	816	THR
1	C	43	LYS
1	C	265	GLU
1	C	378	LEU
1	C	470	GLU
1	C	513	VAL
1	C	773	VAL
1	D	168	ASN
1	D	183	GLN
1	D	296	GLU
1	D	529	VAL
1	D	555	ASN
1	D	601	CYS
1	D	684	GLN
1	D	816	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	161	HIS
1	A	323	GLN
1	A	395	GLN
1	A	525	HIS
1	A	614	HIS
1	A	695	ASN
1	A	798	ASN
1	A	812	HIS
1	A	831	GLN

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Mol	Chain	Res	Type
1	B	68	HIS
1	B	107	GLN
1	B	395	GLN
1	B	424	HIS
1	B	526	HIS
1	B	614	HIS
1	B	742	HIS
1	B	798	ASN
1	B	812	HIS
1	B	831	GLN
1	B	865	HIS
1	C	25	GLN
1	C	614	HIS
1	C	648	GLN
1	C	822	GLN
1	D	39	HIS
1	D	57	GLN
1	D	161	HIS
1	D	226	HIS
1	D	327	GLN
1	D	424	HIS
1	D	562	HIS
1	D	798	ASN
1	D	831	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 oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 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
3	EDO	C	905	-	3,3,3	0.39	0	2,2,2	0.49	0
3	EDO	A	904	-	3,3,3	0.18	0	2,2,2	0.41	0
3	EDO	C	911	-	3,3,3	0.11	0	2,2,2	0.19	0
2	A1INH	B	901	1	16,19,19	0.44	0	16,22,22	0.46	0
3	EDO	A	907	-	3,3,3	0.14	0	2,2,2	0.24	0
3	EDO	B	913	-	3,3,3	0.10	0	2,2,2	0.23	0
3	EDO	C	902	-	3,3,3	0.31	0	2,2,2	0.21	0
3	EDO	A	909	-	3,3,3	0.27	0	2,2,2	0.34	0
3	EDO	A	906	-	3,3,3	0.15	0	2,2,2	0.22	0
3	EDO	A	910	-	3,3,3	0.22	0	2,2,2	0.39	0
3	EDO	D	902	-	3,3,3	0.18	0	2,2,2	0.28	0
3	EDO	C	906	-	3,3,3	0.11	0	2,2,2	0.40	0
3	EDO	A	902	-	3,3,3	0.24	0	2,2,2	0.40	0
2	A1INH	D	901	1	16,19,19	0.39	0	16,22,22	0.35	0
3	EDO	B	909	-	3,3,3	0.14	0	2,2,2	0.25	0
3	EDO	B	911	-	3,3,3	0.19	0	2,2,2	0.36	0
3	EDO	B	907	-	3,3,3	0.18	0	2,2,2	0.29	0
3	EDO	C	908	-	3,3,3	0.12	0	2,2,2	0.27	0
3	EDO	C	910	-	3,3,3	0.14	0	2,2,2	0.16	0
3	EDO	A	905	-	3,3,3	0.21	0	2,2,2	0.30	0
3	EDO	B	908	-	3,3,3	0.14	0	2,2,2	0.15	0
3	EDO	B	912	-	3,3,3	0.26	0	2,2,2	0.39	0
2	A1INH	C	901	1	16,19,19	0.39	0	16,22,22	0.38	0
3	EDO	B	905	-	3,3,3	0.23	0	2,2,2	0.33	0
3	EDO	C	912	-	3,3,3	0.09	0	2,2,2	0.19	0
3	EDO	A	903	-	3,3,3	0.10	0	2,2,2	0.11	0
3	EDO	B	903	-	3,3,3	0.15	0	2,2,2	0.33	0
3	EDO	B	902	-	3,3,3	0.11	0	2,2,2	0.22	0
3	EDO	A	908	-	3,3,3	0.23	0	2,2,2	0.57	0
3	EDO	C	903	-	3,3,3	0.12	0	2,2,2	0.65	0
2	A1INH	A	901	1	16,19,19	0.41	0	16,22,22	0.80	1 (6%)
3	EDO	B	904	-	3,3,3	0.36	0	2,2,2	0.40	0
3	EDO	B	910	-	3,3,3	0.24	0	2,2,2	0.36	0
3	EDO	D	904	-	3,3,3	0.09	0	2,2,2	0.05	0
3	EDO	D	903	-	3,3,3	0.14	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	C	909	-	3,3,3	0.14	0	2,2,2	0.27	0
3	EDO	C	904	-	3,3,3	0.03	0	2,2,2	0.19	0
3	EDO	B	906	-	3,3,3	0.16	0	2,2,2	0.15	0
3	EDO	C	907	-	3,3,3	0.13	0	2,2,2	0.12	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
3	EDO	C	905	-	-	1/1/1/1	-
3	EDO	A	904	-	-	1/1/1/1	-
3	EDO	C	911	-	-	0/1/1/1	-
2	A1INH	B	901	1	-	5/10/14/14	0/1/1/1
3	EDO	A	907	-	-	0/1/1/1	-
3	EDO	B	913	-	-	1/1/1/1	-
3	EDO	C	902	-	-	0/1/1/1	-
3	EDO	A	909	-	-	1/1/1/1	-
3	EDO	A	906	-	-	1/1/1/1	-
3	EDO	A	910	-	-	1/1/1/1	-
3	EDO	D	902	-	-	1/1/1/1	-
3	EDO	C	906	-	-	1/1/1/1	-
3	EDO	A	902	-	-	1/1/1/1	-
2	A1INH	D	901	1	-	3/10/14/14	0/1/1/1
3	EDO	B	909	-	-	1/1/1/1	-
3	EDO	B	911	-	-	0/1/1/1	-
3	EDO	B	907	-	-	0/1/1/1	-
3	EDO	C	908	-	-	1/1/1/1	-
3	EDO	C	910	-	-	1/1/1/1	-
3	EDO	A	905	-	-	1/1/1/1	-
3	EDO	B	908	-	-	1/1/1/1	-
3	EDO	B	912	-	-	0/1/1/1	-
2	A1INH	C	901	1	-	3/10/14/14	0/1/1/1
3	EDO	B	905	-	-	0/1/1/1	-
3	EDO	C	912	-	-	0/1/1/1	-
3	EDO	A	903	-	-	1/1/1/1	-
3	EDO	B	903	-	-	0/1/1/1	-
3	EDO	B	902	-	-	1/1/1/1	-
3	EDO	A	908	-	-	1/1/1/1	-
3	EDO	C	903	-	-	1/1/1/1	-
2	A1INH	A	901	1	-	4/10/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	904	-	-	1/1/1/1	-
3	EDO	B	910	-	-	1/1/1/1	-
3	EDO	D	904	-	-	0/1/1/1	-
3	EDO	D	903	-	-	1/1/1/1	-
3	EDO	C	909	-	-	1/1/1/1	-
3	EDO	C	904	-	-	1/1/1/1	-
3	EDO	B	906	-	-	1/1/1/1	-
3	EDO	C	907	-	-	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(°)
2	A	901	A1INH	C12-S1-C9	-2.70	99.02	104.03

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	A1INH	C3-C4-C5-C6
3	B	902	EDO	O1-C1-C2-O2
3	C	903	EDO	O1-C1-C2-O2
3	C	905	EDO	O1-C1-C2-O2
3	D	902	EDO	O1-C1-C2-O2
2	A	901	A1INH	C2-C3-C4-C5
3	A	904	EDO	O1-C1-C2-O2
3	A	909	EDO	O1-C1-C2-O2
3	B	904	EDO	O1-C1-C2-O2
3	C	909	EDO	O1-C1-C2-O2
3	D	903	EDO	O1-C1-C2-O2
3	A	908	EDO	O1-C1-C2-O2
3	B	910	EDO	O1-C1-C2-O2
3	C	904	EDO	O1-C1-C2-O2
2	B	901	A1INH	C2-C3-C4-C5
2	C	901	A1INH	C2-C3-C4-C5
3	A	902	EDO	O1-C1-C2-O2
3	A	906	EDO	O1-C1-C2-O2
3	B	908	EDO	O1-C1-C2-O2
3	A	905	EDO	O1-C1-C2-O2
3	A	910	EDO	O1-C1-C2-O2
2	B	901	A1INH	C4-C5-C6-C11

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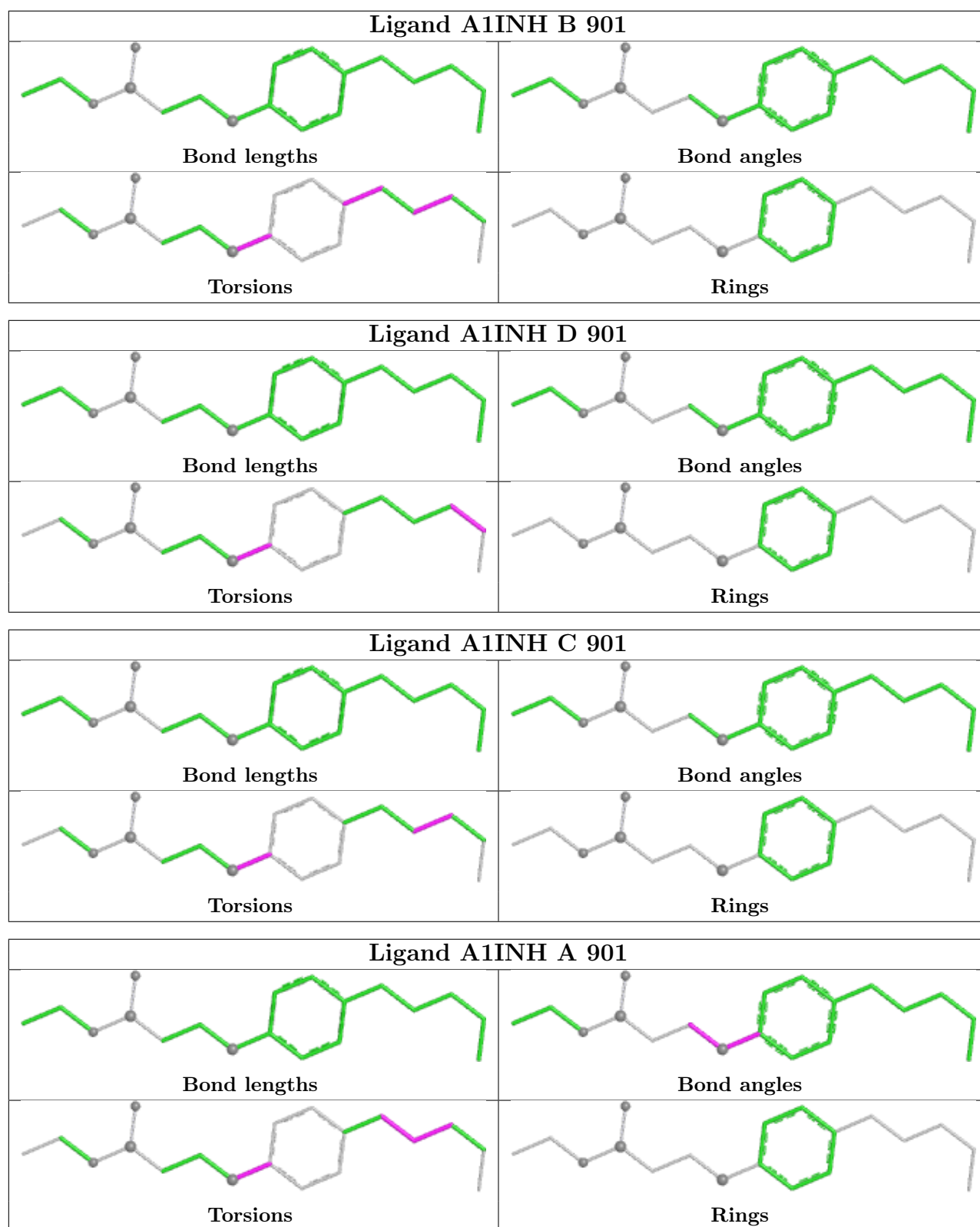
Mol	Chain	Res	Type	Atoms
2	B	901	A1INH	C10-C9-S1-C12
2	B	901	A1INH	C4-C5-C6-C7
3	B	906	EDO	O1-C1-C2-O2
2	A	901	A1INH	C10-C9-S1-C12
2	D	901	A1INH	C8-C9-S1-C12
3	B	913	EDO	O1-C1-C2-O2
3	C	906	EDO	O1-C1-C2-O2
3	C	908	EDO	O1-C1-C2-O2
2	C	901	A1INH	C8-C9-S1-C12
2	D	901	A1INH	C10-C9-S1-C12
2	A	901	A1INH	C8-C9-S1-C12
2	B	901	A1INH	C8-C9-S1-C12
3	A	903	EDO	O1-C1-C2-O2
3	B	909	EDO	O1-C1-C2-O2
3	C	910	EDO	O1-C1-C2-O2
2	C	901	A1INH	C10-C9-S1-C12
2	D	901	A1INH	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	904	EDO	1	0

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



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	816/851 (95%)	-0.15	17 (2%) 63 59	16, 44, 75, 117	36 (4%)
1	B	815/851 (95%)	-0.34	8 (0%) 79 76	12, 37, 71, 114	37 (4%)
1	C	816/851 (95%)	-0.31	11 (1%) 75 71	14, 37, 70, 131	33 (4%)
1	D	798/851 (93%)	0.62	61 (7%) 20 17	29, 65, 115, 148	93 (11%)
All	All	3245/3404 (95%)	-0.05	97 (2%) 52 48	12, 45, 93, 148	199 (6%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	ALA	4.9
1	D	109	LEU	4.7
1	D	86	LEU	4.0
1	D	43	LYS	3.9
1	D	578	SER	3.8
1	D	44	TYR	3.6
1	D	73	TYR	3.5
1	D	78	PRO	3.2
1	D	97	LYS	3.2
1	A	45	SER	3.2
1	D	107	GLN	3.2
1	D	94	LYS	3.1
1	D	265	GLU	3.1
1	D	59	VAL	3.1
1	A	43	LYS	3.0
1	D	215	GLU	3.0
1	B	602	PRO	3.0
1	C	167	LYS	3.0
1	D	61	LYS	3.0
1	D	52	ALA	2.9
1	D	214	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	588	GLN	2.9
1	B	65	SER	2.9
1	D	270	LEU	2.9
1	A	600	SER	2.8
1	D	577	LEU	2.8
1	D	864	HIS	2.8
1	C	112	PHE	2.8
1	D	472	PHE	2.8
1	D	88	TYR	2.7
1	D	535	ALA	2.7
1	D	269	GLY	2.7
1	C	44	TYR	2.7
1	D	303	TYR	2.7
1	D	140	THR	2.7
1	A	21	ALA	2.6
1	A	51	LYS	2.6
1	D	543	THR	2.6
1	D	558	MET	2.6
1	A	167	LYS	2.6
1	D	592	TRP	2.5
1	D	331	VAL	2.5
1	D	174	PRO	2.5
1	D	394	GLU	2.5
1	C	268	GLU	2.5
1	D	483	ILE	2.5
1	A	47	LEU	2.5
1	D	271	LYS	2.5
1	D	58	PHE	2.5
1	C	111	HIS	2.4
1	B	43	LYS	2.4
1	D	79	TYR	2.4
1	A	232	VAL	2.4
1	B	433	SER	2.4
1	C	51	LYS	2.4
1	A	266	GLY	2.4
1	D	575	TYR	2.4
1	D	93	LYS	2.4
1	A	434	GLU	2.3
1	D	580	PRO	2.3
1	D	476	GLU	2.3
1	D	533	GLU	2.3
1	D	579	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	380	LEU	2.2
1	D	397	LEU	2.2
1	D	603	PRO	2.2
1	D	168	ASN	2.2
1	D	396	ARG	2.2
1	D	95	VAL	2.2
1	D	85	SER	2.2
1	A	137	PHE	2.2
1	A	95	VAL	2.1
1	D	330	ILE	2.1
1	D	329	LYS	2.1
1	D	534	ALA	2.1
1	B	50	ASN	2.1
1	B	168	ASN	2.1
1	B	98	GLU	2.1
1	C	45	SER	2.1
1	D	146	SER	2.1
1	D	171	MET	2.1
1	D	750	ALA	2.1
1	D	501	GLY	2.1
1	D	576	LYS	2.1
1	B	841	SER	2.1
1	D	189	MET	2.1
1	D	574	VAL	2.1
1	D	749	VAL	2.1
1	D	604	ASP	2.1
1	C	22	ALA	2.0
1	A	231[A]	ASN	2.0
1	C	98	GLU	2.0
1	A	635	LYS	2.0
1	C	166	GLY	2.0
1	A	602	PRO	2.0
1	A	44	TYR	2.0
1	A	303	TYR	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	B	902	4/4	0.77	0.20	79,80,81,84	0
3	EDO	B	912	4/4	0.81	0.17	60,64,66,68	0
3	EDO	A	910	4/4	0.84	0.17	69,78,80,82	0
3	EDO	C	912	4/4	0.86	0.16	59,64,65,66	0
3	EDO	D	902	4/4	0.86	0.18	55,58,59,59	0
3	EDO	B	904	4/4	0.87	0.15	47,52,52,53	0
3	EDO	C	902	4/4	0.88	0.15	46,46,49,49	0
3	EDO	C	903	4/4	0.88	0.15	52,54,54,54	0
3	EDO	D	903	4/4	0.88	0.14	55,60,65,67	0
3	EDO	C	904	4/4	0.90	0.12	45,46,48,48	0
3	EDO	A	909	4/4	0.90	0.15	59,63,64,66	0
3	EDO	B	907	4/4	0.92	0.12	54,55,56,58	0
3	EDO	C	910	4/4	0.92	0.14	56,62,67,68	0
3	EDO	A	904	4/4	0.92	0.09	48,48,48,49	0
3	EDO	A	907	4/4	0.92	0.17	54,58,67,71	0
3	EDO	A	902	4/4	0.92	0.12	57,57,59,59	0
3	EDO	B	910	4/4	0.93	0.13	59,63,69,76	0
3	EDO	A	908	4/4	0.93	0.12	60,64,66,67	0
2	A1INH	D	901	19/19	0.93	0.13	48,87,97,97	3
3	EDO	D	904	4/4	0.93	0.16	70,71,71,73	0
3	EDO	C	909	4/4	0.94	0.11	44,47,50,53	0
3	EDO	B	908	4/4	0.94	0.14	60,63,63,70	0
3	EDO	C	905	4/4	0.94	0.11	50,54,54,56	0
4	CL	A	911	1/1	0.94	0.09	53,53,53,53	0
3	EDO	B	909	4/4	0.95	0.08	47,51,52,52	0
3	EDO	B	903	4/4	0.95	0.09	40,43,45,45	0
3	EDO	B	911	4/4	0.95	0.08	50,55,57,60	0
3	EDO	C	908	4/4	0.96	0.08	42,44,45,45	0
2	A1INH	B	901	19/19	0.96	0.12	29,86,101,105	4
3	EDO	B	906	4/4	0.96	0.08	37,38,41,43	0
3	EDO	A	903	4/4	0.96	0.07	41,42,45,48	0
2	A1INH	C	901	19/19	0.96	0.12	33,71,83,87	3

*Continued on next page...*

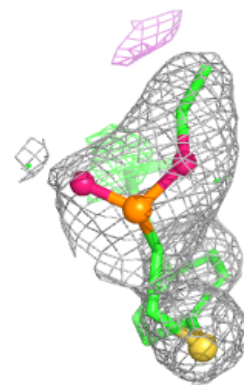
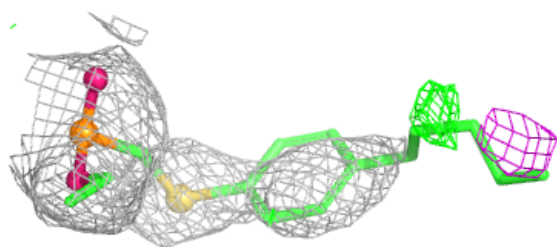
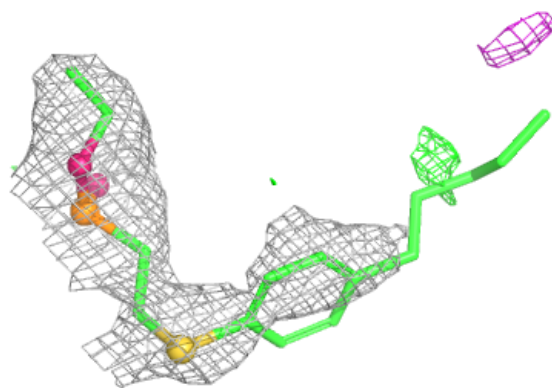
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	905	4/4	0.96	0.07	38,40,40,40	0
2	A1INH	A	901	19/19	0.96	0.13	42,74,86,89	0
3	EDO	C	906	4/4	0.96	0.07	35,37,40,42	0
4	CL	C	913	1/1	0.96	0.07	46,46,46,46	0
3	EDO	C	907	4/4	0.97	0.08	41,41,42,42	0
3	EDO	C	911	4/4	0.97	0.08	39,40,40,43	0
3	EDO	B	913	4/4	0.97	0.12	53,56,56,56	0
3	EDO	B	905	4/4	0.97	0.07	42,42,43,43	0
3	EDO	A	906	4/4	0.98	0.08	58,58,60,63	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.

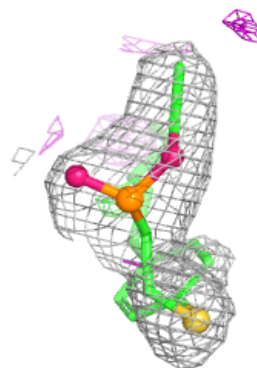
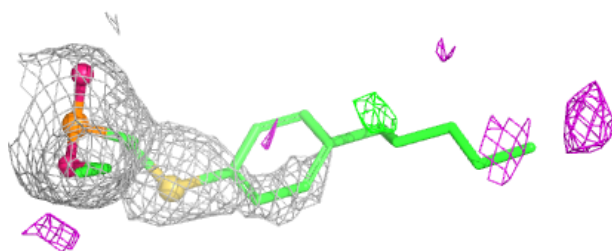
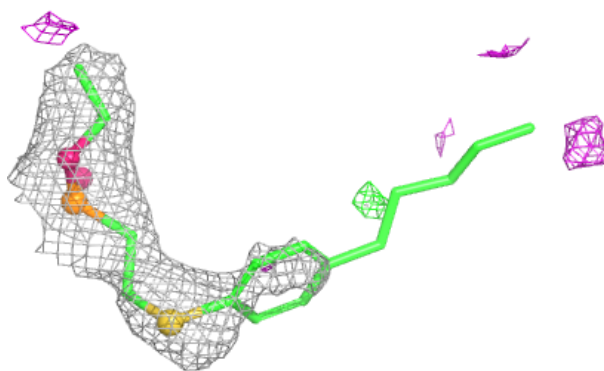
**Electron density around A1INH D 901:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

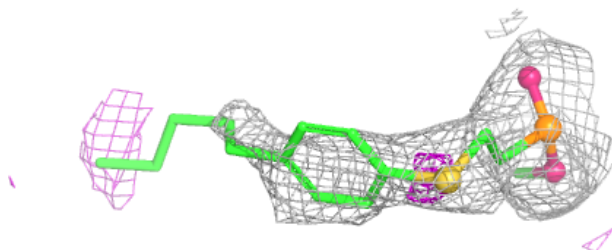
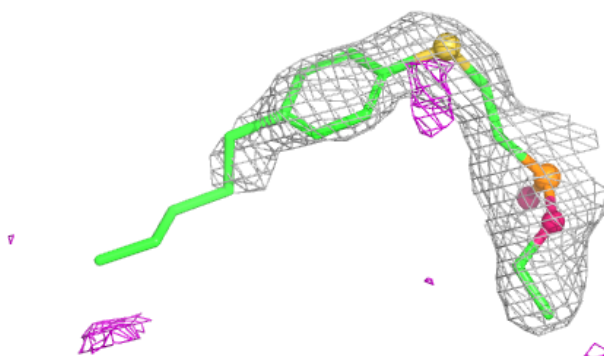


**Electron density around A1INH B 901:**

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

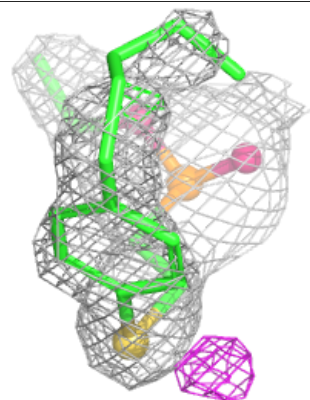
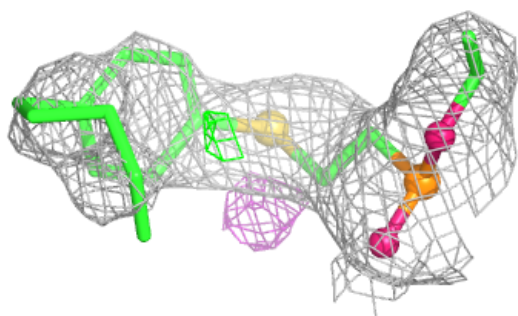
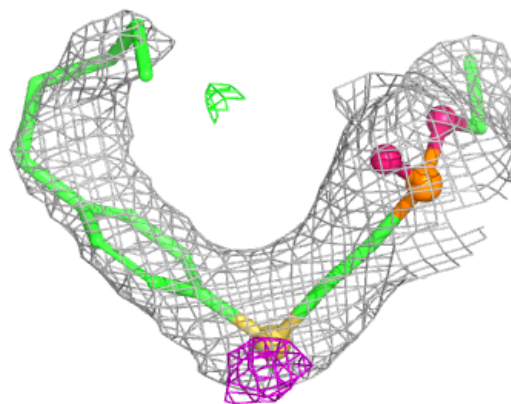
**Electron density around A1INH C 901:**

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



**Electron density around A1INH A 901:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.