



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:29 PM UTC

PDB ID : 7NBG / pdb_00007nbg
Title : Crystal structure of human serine racemase in complex with DSiP fragment
Z52314092, XChem fragment screen.
Authors : Koulouris, C.R.; Roe, S.M.
Deposited on : 2021-01-26
Resolution : 1.53 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

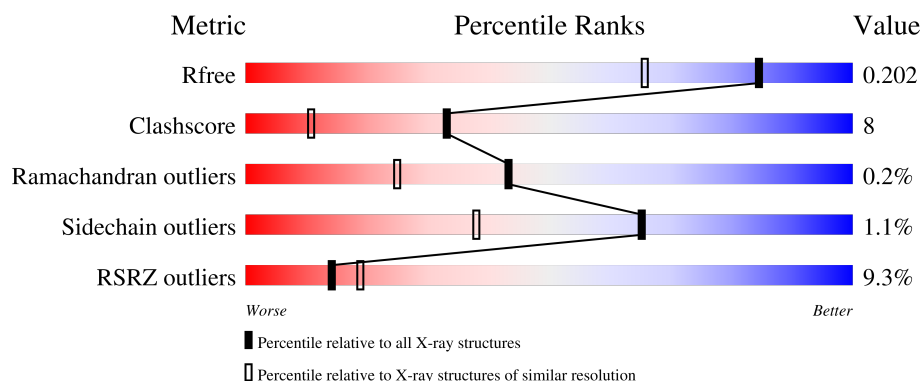
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	AAA	346	8% 82% 11% 7%
1	BBB	346	12% 82% 8% 11%
1	CCC	346	4% 81% 10% 8%
1	DDD	346	10% 76% 13% 10%

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
6	GOL	AAA	413[A]	-	-	X	-
6	GOL	CCC	402	-	-	X	-
6	GOL	DDD	411[A]	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11577 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 Serine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	322	Total	C	N	O	S	0	36	0
			2716	1725	461	518	12			
1	BBB	308	Total	C	N	O	S	9	21	0
			2437	1554	407	465	11			
1	CCC	317	Total	C	N	O	S	0	33	0
			2648	1691	436	509	12			
1	DDD	310	Total	C	N	O	S	0	39	0
			2572	1637	426	495	14			

There are 32 discrepancies between the modelled and reference sequences:

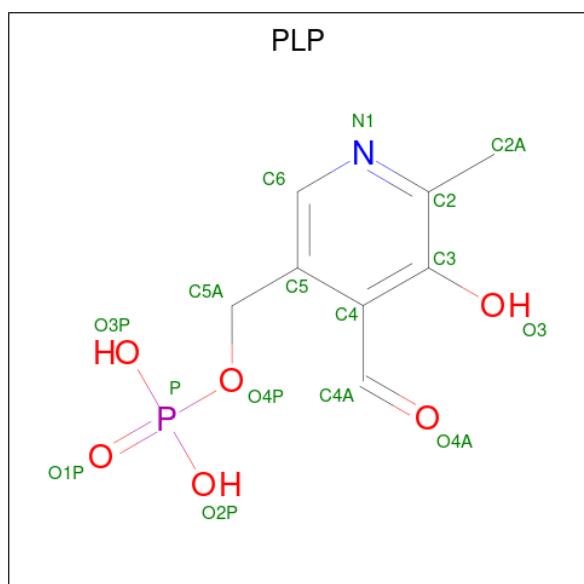
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	6	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	341	HIS	-	expression tag	UNP Q9GZT4
AAA	342	HIS	-	expression tag	UNP Q9GZT4
AAA	343	HIS	-	expression tag	UNP Q9GZT4
AAA	344	HIS	-	expression tag	UNP Q9GZT4
AAA	345	HIS	-	expression tag	UNP Q9GZT4
AAA	346	HIS	-	expression tag	UNP Q9GZT4
BBB	2	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	6	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	341	HIS	-	expression tag	UNP Q9GZT4
BBB	342	HIS	-	expression tag	UNP Q9GZT4
BBB	343	HIS	-	expression tag	UNP Q9GZT4
BBB	344	HIS	-	expression tag	UNP Q9GZT4
BBB	345	HIS	-	expression tag	UNP Q9GZT4
BBB	346	HIS	-	expression tag	UNP Q9GZT4
CCC	2	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	6	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	341	HIS	-	expression tag	UNP Q9GZT4
CCC	342	HIS	-	expression tag	UNP Q9GZT4
CCC	343	HIS	-	expression tag	UNP Q9GZT4

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	344	HIS	-	expression tag	UNP Q9GZT4
CCC	345	HIS	-	expression tag	UNP Q9GZT4
CCC	346	HIS	-	expression tag	UNP Q9GZT4
DDD	2	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	6	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	341	HIS	-	expression tag	UNP Q9GZT4
DDD	342	HIS	-	expression tag	UNP Q9GZT4
DDD	343	HIS	-	expression tag	UNP Q9GZT4
DDD	344	HIS	-	expression tag	UNP Q9GZT4
DDD	345	HIS	-	expression tag	UNP Q9GZT4
DDD	346	HIS	-	expression tag	UNP Q9GZT4

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	1
			30	16	2	10	2		
2	BBB	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	CCC	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	DDD	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	1
			8	4	4		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	1
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	1
			8	4	4		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		

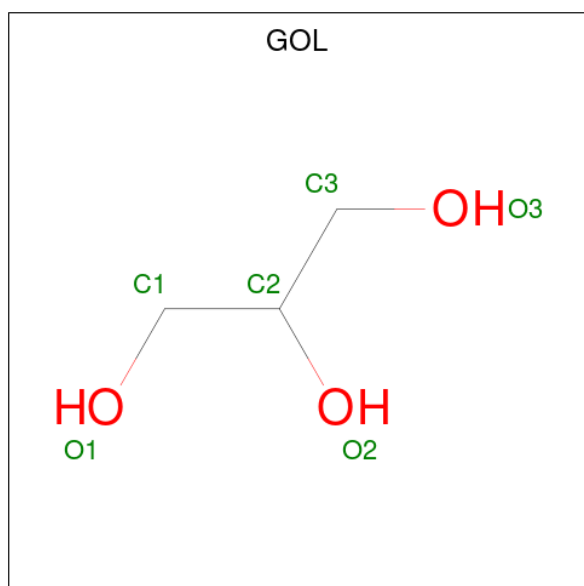
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	4	Total	Na	0	1
			5	5		
4	BBB	2	Total	Na	0	0
			2	2		
4	CCC	2	Total	Na	0	0
			2	2		
4	DDD	1	Total	Na	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Ca	0	0
			1	1		
5	BBB	1	Total	Ca	0	0
			1	1		
5	CCC	1	Total	Ca	0	1
			2	2		
5	DDD	1	Total	Ca	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



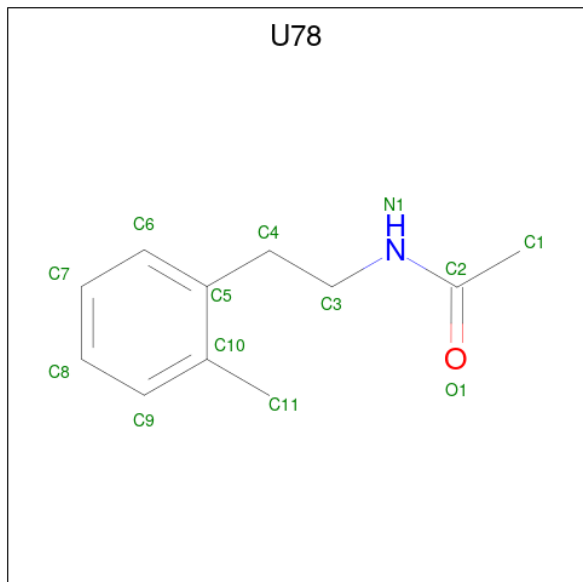
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	1
			6	3	3		
6	CCC	1	Total	C	O	0	0
			6	3	3		
6	CCC	1	Total	C	O	0	0
			6	3	3		
6	CCC	1	Total	C	O	0	1
			12	6	6		
6	DDD	1	Total	C	O	0	1
			12	6	6		

- Molecule 7 is {N}-[2-(2-methylphenyl)ethyl]ethanamide (CCD ID: U78) (formula: C₁₁H₁₅NO) (labeled as "Ligand of Interest" by depositor).

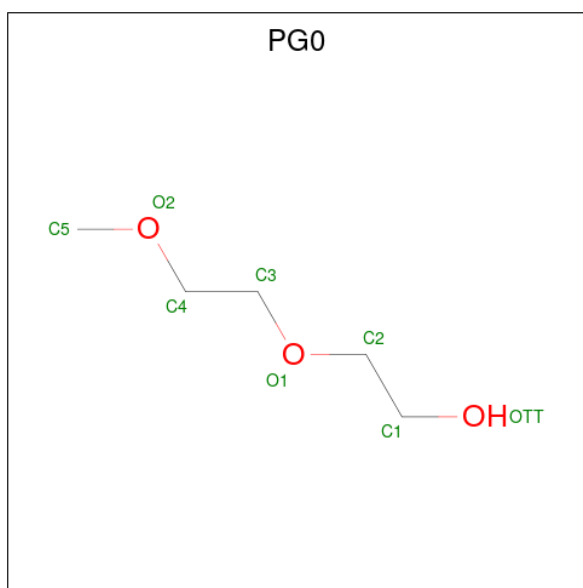


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	AAA	1	Total	C	N	O	0	0
			13	11	1	1		
7	BBB	1	Total	C	N	O	0	0
			13	11	1	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

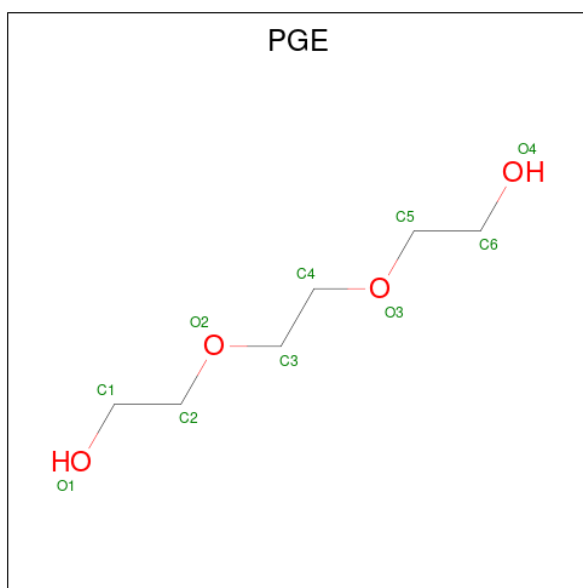
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	BBB	1	Total	Mg	0	0
			1	1		
8	DDD	1	Total	Mg	0	0
			1	1		

- Molecule 9 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



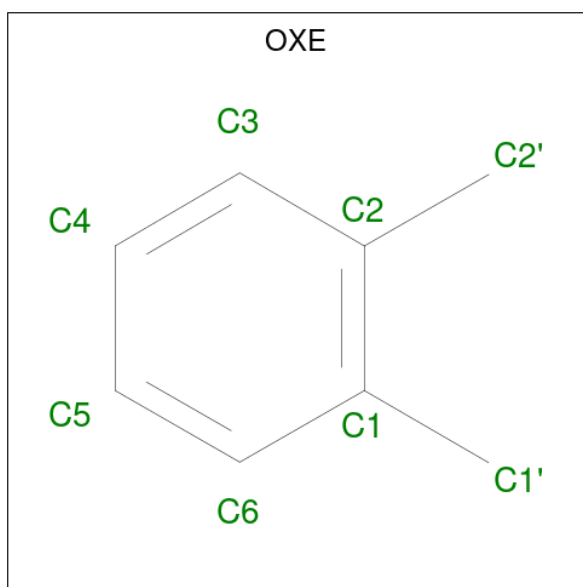
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	DDD	1	Total	C	O	0	0
			8	5	3		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	DDD	1	Total	C	O	0	0
			10	6	4		

- Molecule 11 is ORTHO-XYLENE (CCD ID: OXE) (formula: C_8H_{10}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	DDD	1	Total C 8 8	0	1

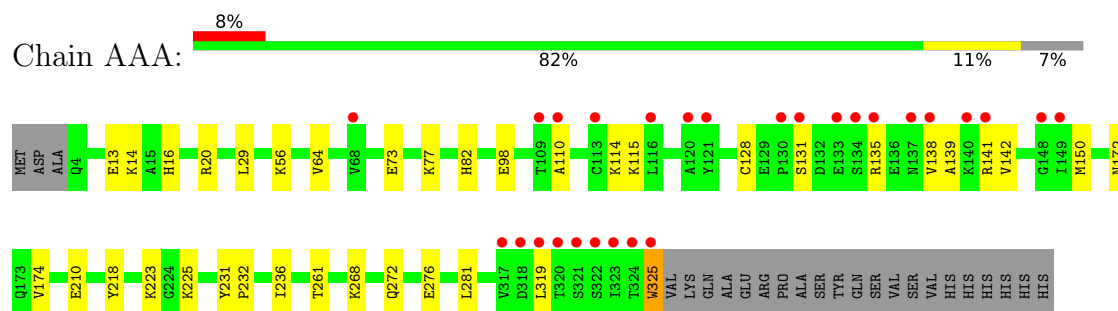
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	AAA	295	Total O 299 299	0	6
12	BBB	157	Total O 158 158	0	1
12	CCC	236	Total O 237 237	0	2
12	DDD	253	Total O 254 254	0	5

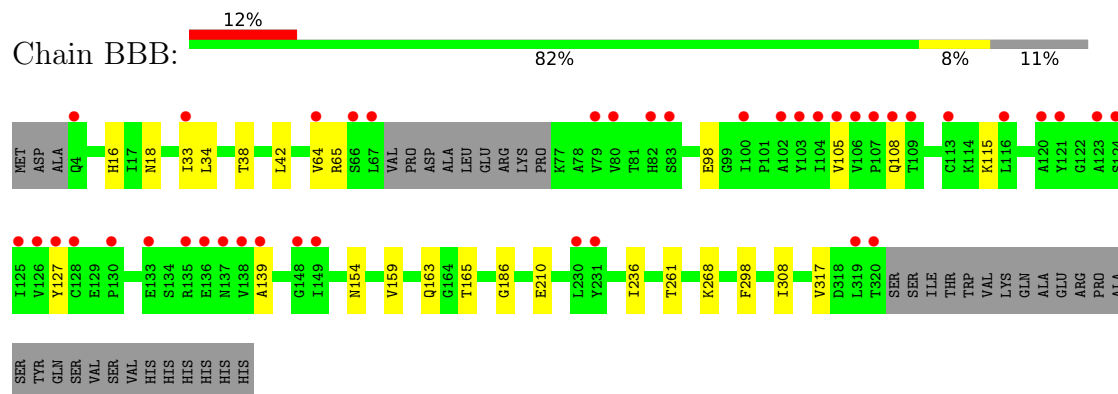
3 Residue-property plots [i](#)

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.

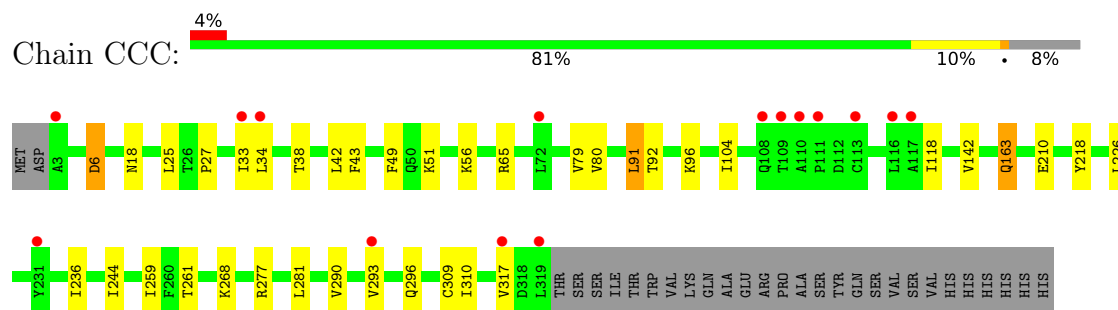
- Molecule 1: Serine racemase



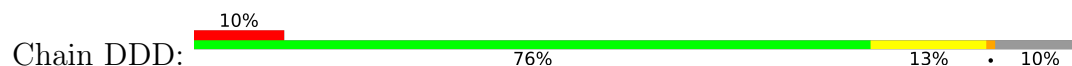
- Molecule 1: Serine racemase

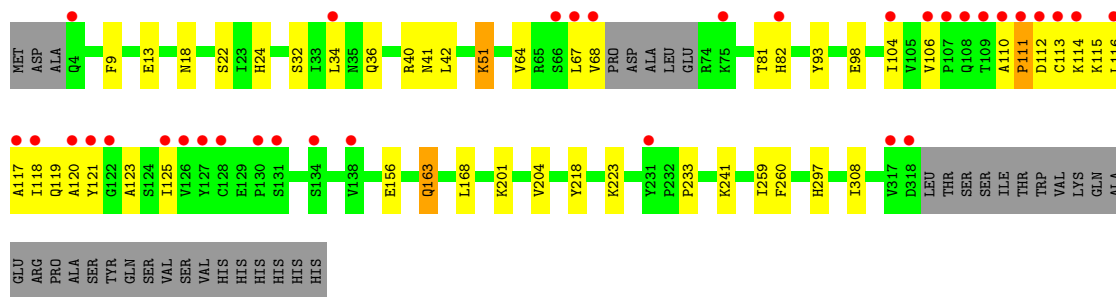


- Molecule 1: Serine racemase



- Molecule 1: Serine racemase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.11Å 154.76Å 85.40Å 90.00° 98.14° 90.00°	Depositor
Resolution (Å)	77.38 – 1.53 77.38 – 1.53	Depositor EDS
% Data completeness (in resolution range)	95.8 (77.38-1.53) 95.8 (77.38-1.53)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.202 0.182 , 0.202	Depositor DCC
R_{free} test set	8706 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11577	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.23% 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: CA, PG0, PGE, GOL, PLP, U78, MG, OXE, EDO, NA

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	AAA	0.46	0/2765	0.81	0/3761
1	BBB	0.46	0/2479	0.83	0/3382
1	CCC	0.46	0/2694	0.81	1/3681 (0.0%)
1	DDD	0.46	0/2616	0.80	1/3571 (0.0%)
All	All	0.46	0/10554	0.81	2/14395 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	163	GLN	CB-CG-CD	7.83	125.92	112.60
1	DDD	163	GLN	CB-CG-CD	7.47	125.31	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	AAA	2716	0	2714	40	0
1	BBB	2437	0	2410	16	0
1	CCC	2648	0	2622	33	0
1	DDD	2572	0	2520	72	0
2	AAA	30	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	15	0	6	0	0
2	CCC	15	0	6	1	0
2	DDD	15	0	6	0	0
3	AAA	24	0	36	1	0
3	BBB	4	0	6	0	0
3	CCC	20	0	30	2	0
3	DDD	16	0	24	0	0
4	AAA	5	0	0	0	0
4	BBB	2	0	0	0	0
4	CCC	2	0	0	0	0
4	DDD	1	0	0	0	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	2	0	0	1	0
5	DDD	1	0	0	0	0
6	AAA	12	0	16	9	0
6	CCC	24	0	32	6	0
6	DDD	12	0	16	8	0
7	AAA	13	0	0	0	0
7	BBB	13	0	0	0	0
8	BBB	1	0	0	0	0
8	DDD	1	0	0	0	0
9	DDD	8	0	12	1	0
10	DDD	10	0	14	3	0
11	DDD	8	0	10	0	0
12	AAA	299	0	0	9	0
12	BBB	158	0	0	3	0
12	CCC	237	0	0	4	0
12	DDD	254	0	0	9	1
All	All	11577	0	10492	166	1

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 8.

All (166) 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:DDD:18[B]:ASN:OD1	1:DDD:67[B]:LEU:HB2	1.28	1.33
1:DDD:112[A]:ASP:O	1:DDD:114[A]:LYS:N	1.62	1.27
1:DDD:67[B]:LEU:CD2	1:DDD:68[B]:VAL:HG23	1.66	1.25
1:DDD:67[B]:LEU:HD23	1:DDD:68[B]:VAL:HG23	1.27	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:117[B]:ALA:O	1:DDD:120[B]:ALA:HB3	1.50	1.07
1:DDD:18[B]:ASN:OD1	1:DDD:67[B]:LEU:CB	2.03	1.06
1:DDD:18[B]:ASN:CG	1:DDD:67[B]:LEU:HB2	1.84	1.01
6:DDD:411[A]:GOL:H31	12:DDD:530:HOH:O	1.61	0.98
1:AAA:16[A]:HIS:ND1	12:AAA:501[A]:HOH:O	1.95	0.97
1:AAA:261:THR:H	6:AAA:413[A]:GOL:H32	1.29	0.97
1:BBB:108:GLN:HA	12:BBB:591:HOH:O	1.65	0.95
1:DDD:156:GLU:OE2	12:DDD:501:HOH:O	1.86	0.94
1:DDD:223:LYS:HG2	12:DDD:511:HOH:O	1.69	0.91
1:AAA:139:ALA:HB1	1:AAA:150[A]:MET:HE1	1.54	0.90
1:AAA:16[A]:HIS:CE1	12:AAA:501[A]:HOH:O	2.25	0.88
1:DDD:297:HIS:CD2	6:DDD:411[A]:GOL:H12	2.09	0.88
1:DDD:67[B]:LEU:HD23	1:DDD:68[B]:VAL:CG2	2.05	0.85
1:DDD:112[A]:ASP:C	1:DDD:114[A]:LYS:H	1.86	0.82
1:DDD:241:LYS:HB3	10:DDD:409:PGE:H22	1.61	0.82
6:AAA:413[A]:GOL:H31	12:AAA:687:HOH:O	1.80	0.82
1:DDD:117[B]:ALA:O	1:DDD:120[B]:ALA:CB	2.29	0.81
1:DDD:67[B]:LEU:CD2	1:DDD:68[B]:VAL:CG2	2.57	0.80
1:DDD:67[B]:LEU:HD23	1:DDD:67[B]:LEU:C	2.08	0.79
1:DDD:112[A]:ASP:C	1:DDD:114[A]:LYS:N	2.41	0.76
1:DDD:36[B]:GLN:HE21	1:DDD:36[B]:GLN:HA	1.50	0.75
1:DDD:36[B]:GLN:HA	1:DDD:36[B]:GLN:NE2	2.03	0.74
1:CCC:51:LYS:HE3	12:CCC:510:HOH:O	1.86	0.74
6:AAA:413[A]:GOL:H12	12:AAA:531:HOH:O	1.88	0.73
1:DDD:116[B]:LEU:O	1:DDD:120[B]:ALA:HB2	1.88	0.73
1:DDD:81:THR:CG2	1:DDD:104:ILE:HD13	2.19	0.72
1:AAA:261:THR:H	6:AAA:413[A]:GOL:C3	2.03	0.70
1:DDD:18[B]:ASN:ND2	1:DDD:67[B]:LEU:HB2	2.05	0.70
1:AAA:114[A]:LYS:HB2	1:AAA:114[A]:LYS:NZ	2.08	0.68
1:DDD:67[B]:LEU:HD22	1:DDD:68[B]:VAL:HG23	1.69	0.68
1:CCC:79[B]:VAL:HG11	1:CCC:91:LEU:HG	1.76	0.67
1:DDD:112[A]:ASP:O	1:DDD:113[A]:CYS:C	2.39	0.64
1:DDD:260:PHE:HA	6:DDD:411[A]:GOL:O3	1.97	0.64
1:CCC:293[A]:VAL:HG21	1:CCC:310:ILE:HD11	1.80	0.64
1:DDD:51[B]:LYS:HE3	1:DDD:93:TYR:OH	1.99	0.63
1:AAA:114[A]:LYS:HB2	1:AAA:114[A]:LYS:HZ3	1.61	0.63
5:CCC:403[B]:CA:CA	12:CCC:556:HOH:O	1.75	0.63
1:AAA:231[B]:TYR:CD1	12:AAA:677[B]:HOH:O	2.50	0.60
1:CCC:49:PHE:HB3	6:CCC:402:GOL:H2	1.83	0.59
1:DDD:118[B]:ILE:HA	1:DDD:121[B]:TYR:CE2	2.37	0.59
1:DDD:32:SER:O	1:DDD:36[A]:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:139:ALA:HB1	1:AAA:150[A]:MET:CE	2.28	0.58
1:DDD:41[B]:ASN:ND2	12:DDD:506:HOH:O	2.36	0.57
1:BBB:236[A]:ILE:HD13	1:BBB:268:LYS:CG	2.34	0.57
1:AAA:131[A]:SER:O	1:AAA:135[A]:ARG:HG3	2.04	0.57
1:DDD:114[B]:LYS:O	1:DDD:118[B]:ILE:HG13	2.06	0.56
1:DDD:117[B]:ALA:C	1:DDD:120[B]:ALA:HB3	2.26	0.56
1:DDD:22:SER:O	1:DDD:51[B]:LYS:HD2	2.05	0.56
1:AAA:261:THR:N	6:AAA:413[A]:GOL:H32	2.10	0.56
1:CCC:33[A]:ILE:HG23	1:CCC:34:LEU:HD12	1.88	0.56
1:CCC:218:TYR:HA	1:CCC:259[A]:ILE:HG21	1.89	0.55
1:BBB:105:VAL:HG21	1:BBB:139:ALA:HA	1.90	0.54
1:AAA:236[B]:ILE:HD13	1:AAA:268:LYS:HG3	1.90	0.54
1:CCC:6:ASP:OD1	3:CCC:404:EDO:H12	2.07	0.54
1:AAA:236[B]:ILE:HD13	1:AAA:268:LYS:CG	2.38	0.54
1:DDD:118[B]:ILE:C	1:DDD:120[B]:ALA:N	2.62	0.53
1:DDD:24:HIS:CD2	1:DDD:51[A]:LYS:HD2	2.44	0.53
1:AAA:64:VAL:HG12	1:AAA:98:GLU:HG3	1.91	0.52
1:DDD:24:HIS:CE1	1:DDD:51[A]:LYS:HE3	2.45	0.52
1:DDD:233:PRO:HD2	10:DDD:409:PGE:H2	1.92	0.51
1:AAA:172:ASN:ND2	12:DDD:505:HOH:O	2.44	0.51
1:DDD:18[B]:ASN:OD1	1:DDD:67[B]:LEU:CG	2.58	0.51
1:BBB:115:LYS:HE2	12:BBB:591:HOH:O	2.11	0.50
1:DDD:18[B]:ASN:HD21	1:DDD:67[B]:LEU:HB2	1.77	0.50
1:DDD:34[A]:LEU:HB3	1:DDD:42:LEU:HD12	1.93	0.50
1:DDD:81:THR:HG23	1:DDD:104:ILE:HD13	1.94	0.50
1:DDD:82[B]:HIS:HD2	9:DDD:404:PG0:H12	1.77	0.50
1:CCC:79[A]:VAL:HG21	1:CCC:91:LEU:HG	1.93	0.49
1:CCC:236[B]:ILE:CD1	1:CCC:268:LYS:HG3	2.41	0.49
1:DDD:218:TYR:HE1	6:DDD:411[B]:GOL:H12	1.76	0.49
1:AAA:231[B]:TYR:HD1	12:AAA:677[B]:HOH:O	1.92	0.49
1:AAA:232[B]:PRO:HA	6:AAA:410:GOL:H32	1.94	0.49
1:AAA:272[B]:GLN:O	1:AAA:276[B]:GLU:HG3	2.12	0.49
1:CCC:18[C]:ASN:HD21	1:CCC:65:ARG:HB2	1.77	0.49
1:DDD:259:ILE:O	6:DDD:411[A]:GOL:H11	2.13	0.49
1:DDD:118[B]:ILE:O	1:DDD:121[B]:TYR:N	2.43	0.49
1:DDD:117[B]:ALA:O	1:DDD:120[B]:ALA:N	2.46	0.48
1:AAA:236[B]:ILE:CD1	1:AAA:268:LYS:HG3	2.44	0.48
6:DDD:411[A]:GOL:C3	12:DDD:530:HOH:O	2.38	0.48
1:DDD:201:LYS:HG2	1:DDD:204:VAL:HG23	1.95	0.48
1:CCC:18[C]:ASN:HD21	1:CCC:65:ARG:CB	2.26	0.48
1:CCC:18[C]:ASN:ND2	1:CCC:65:ARG:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:277[A]:ARG:NE	12:CCC:504:HOH:O	2.46	0.47
1:DDD:67[B]:LEU:CD2	1:DDD:67[B]:LEU:C	2.81	0.47
1:AAA:14[B]:LYS:HG3	12:AAA:634:HOH:O	2.13	0.47
1:DDD:13[A]:GLU:OE2	12:DDD:502:HOH:O	2.20	0.47
1:DDD:110[B]:ALA:O	1:DDD:111[B]:PRO:O	2.33	0.47
1:AAA:232[A]:PRO:HA	6:AAA:410:GOL:H32	1.95	0.47
1:DDD:9[B]:PHE:CE1	1:DDD:168[B]:LEU:HD21	2.50	0.47
1:DDD:118[B]:ILE:C	1:DDD:120[B]:ALA:H	2.21	0.47
1:DDD:117[B]:ALA:O	1:DDD:120[B]:ALA:CA	2.63	0.46
1:DDD:110[B]:ALA:HB1	1:DDD:111[B]:PRO:HD2	1.98	0.46
1:BBB:210:GLU:O	1:BBB:261:THR:HA	2.15	0.46
1:CCC:104:ILE:HG21	1:CCC:118:ILE:HG21	1.97	0.46
1:DDD:297:HIS:NE2	6:DDD:411[A]:GOL:H12	2.30	0.46
1:AAA:138:VAL:O	1:AAA:142:VAL:HG23	2.16	0.46
1:CCC:226:LEU:CD1	1:CCC:244[B]:ILE:HG13	2.45	0.46
1:BBB:127:TYR:CD1	12:BBB:591:HOH:O	2.56	0.46
1:CCC:290:VAL:O	1:CCC:293[B]:VAL:HG12	2.15	0.46
1:BBB:34[A]:LEU:HD23	1:BBB:34[A]:LEU:N	2.31	0.45
1:AAA:64:VAL:CG1	1:AAA:98:GLU:HG3	2.46	0.45
1:DDD:40:ARG:HD2	1:DDD:308:ILE:CD1	2.46	0.45
1:AAA:218:TYR:CE1	6:AAA:413[A]:GOL:H11	2.51	0.45
1:AAA:128:CYS:SG	1:AAA:135[A]:ARG:HG2	2.57	0.45
1:CCC:236[B]:ILE:HD13	1:CCC:268:LYS:CG	2.47	0.44
1:CCC:259[A]:ILE:CG2	6:CCC:409[A]:GOL:H2	2.47	0.44
1:DDD:114[B]:LYS:O	1:DDD:117[B]:ALA:HB3	2.18	0.44
1:AAA:281[B]:LEU:HD21	1:CCC:281[B]:LEU:HD13	2.00	0.44
1:BBB:16[A]:HIS:CD2	1:BBB:165:THR:HB	2.52	0.44
1:AAA:174:VAL:HG13	3:AAA:406[A]:EDO:H22	2.00	0.44
1:AAA:110:ALA:O	1:AAA:115:LYS:HE3	2.17	0.44
1:DDD:114[B]:LYS:HA	1:DDD:117[B]:ALA:HB3	2.00	0.44
1:AAA:210:GLU:O	1:AAA:261:THR:HA	2.18	0.43
1:DDD:36[B]:GLN:NE2	1:DDD:36[B]:GLN:CA	2.73	0.43
1:BBB:105:VAL:HG21	1:BBB:139:ALA:CA	2.48	0.43
1:CCC:80:VAL:HG11	1:CCC:142[B]:VAL:HG13	2.01	0.43
1:CCC:236[B]:ILE:HD13	1:CCC:268:LYS:HG3	2.00	0.43
1:DDD:118[B]:ILE:HB	1:DDD:125:ILE:HD11	2.01	0.43
1:AAA:82[B]:HIS:CE1	1:AAA:135[B]:ARG:HG2	2.54	0.43
1:AAA:261:THR:OG1	6:AAA:413[A]:GOL:H32	2.18	0.43
1:CCC:49:PHE:CB	6:CCC:402:GOL:H2	2.48	0.43
1:CCC:92:THR:O	1:CCC:96:LYS:HG2	2.19	0.43
1:DDD:32:SER:O	1:DDD:36[B]:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:67[B]:LEU:HD23	1:DDD:68[B]:VAL:N	2.34	0.43
1:CCC:210[A]:GLU:O	1:CCC:261:THR:HA	2.19	0.43
1:AAA:281[A]:LEU:HD11	1:AAA:319:LEU:HD11	2.00	0.42
1:BBB:38:THR:HG21	1:BBB:42:LEU:HD11	2.00	0.42
1:AAA:29:LEU:HB3	6:CCC:402:GOL:H32	2.02	0.42
1:AAA:82[A]:HIS:HD2	12:AAA:552:HOH:O	2.02	0.42
1:CCC:38:THR:HG21	1:CCC:42:LEU:HD11	2.01	0.42
1:CCC:27[B]:PRO:HD3	6:CCC:402:GOL:O2	2.19	0.42
1:DDD:18[B]:ASN:OD1	1:DDD:67[B]:LEU:CA	2.66	0.42
1:CCC:27[A]:PRO:HD3	6:CCC:402:GOL:O2	2.19	0.42
1:CCC:56:LYS:NZ	2:CCC:401:PLP:O3	2.51	0.42
1:DDD:40:ARG:HD2	1:DDD:308:ILE:HD11	2.02	0.42
1:BBB:64:VAL:HG12	1:BBB:98:GLU:HG3	2.01	0.42
1:DDD:218:TYR:CE1	6:DDD:411[B]:GOL:H12	2.54	0.42
1:AAA:73[A]:GLU:HG2	1:AAA:77[A]:LYS:HE3	2.02	0.42
1:AAA:223[B]:LYS:HG3	1:AAA:225:LYS:HG2	2.02	0.41
1:CCC:293[A]:VAL:HG21	1:CCC:310:ILE:CD1	2.49	0.41
1:DDD:51[B]:LYS:CB	1:DDD:51[B]:LYS:NZ	2.82	0.41
1:AAA:56[A]:LYS:NZ	2:AAA:401[A]:PLP:O3	2.50	0.41
1:DDD:112[A]:ASP:O	1:DDD:114[A]:LYS:CA	2.59	0.41
1:BBB:33:ILE:HG22	1:BBB:34[A]:LEU:HD23	2.02	0.41
1:DDD:112[A]:ASP:O	1:DDD:115[A]:LYS:N	2.49	0.41
1:AAA:272[B]:GLN:HG3	1:AAA:325:TRP:HZ2	1.84	0.41
1:CCC:296[B]:GLN:HG2	12:CCC:656:HOH:O	2.20	0.41
1:DDD:168[A]:LEU:HD21	12:DDD:505:HOH:O	2.21	0.41
1:AAA:231[B]:TYR:CE1	12:AAA:677[B]:HOH:O	2.73	0.41
1:BBB:18[A]:ASN:HD21	1:BBB:65:ARG:CB	2.34	0.41
1:BBB:298:PHE:CE1	1:BBB:308[A]:ILE:HD13	2.56	0.41
10:DDD:409:PGE:H5	12:DDD:588:HOH:O	2.20	0.41
1:CCC:6:ASP:OD1	3:CCC:404:EDO:C1	2.69	0.40
1:DDD:104:ILE:HG12	1:DDD:123[B]:ALA:HB1	2.03	0.40
1:DDD:117[B]:ALA:C	1:DDD:120[B]:ALA:H	2.29	0.40
1:BBB:159:VAL:O	1:BBB:163:GLN:HG2	2.22	0.40
1:CCC:25[B]:LEU:CD1	1:CCC:25[B]:LEU:C	2.94	0.40
1:DDD:51[B]:LYS:CB	1:DDD:51[B]:LYS:HZ2	2.34	0.40
1:CCC:43:PHE:O	1:CCC:309:CYS:HA	2.21	0.40
1:DDD:64:VAL:HG12	1:DDD:98:GLU:HG3	2.03	0.40
1:AAA:13[B]:GLU:O	1:AAA:16[B]:HIS:HB3	2.22	0.40
1:BBB:154:ASN:CG	1:BBB:186:GLY:HA3	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:DDD:516:HOH:O	12:DDD:596:HOH:O[1_655]	1.99	0.21

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	AAA	357/346 (103%)	350 (98%)	7 (2%)	0	100	100
1	BBB	325/346 (94%)	320 (98%)	5 (2%)	0	100	100
1	CCC	351/346 (101%)	346 (99%)	5 (1%)	0	100	100
1	DDD	343/346 (99%)	331 (96%)	8 (2%)	4 (1%)	10	1
All	All	1376/1384 (99%)	1347 (98%)	25 (2%)	4 (0%)	43	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	111[A]	PRO
1	DDD	111[B]	PRO
1	DDD	119[A]	GLN
1	DDD	119[B]	GLN

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	AAA	296/291 (102%)	292 (99%)	4 (1%)	59	29
1	BBB	258/291 (89%)	257 (100%)	1 (0%)	84	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CCC	284/291 (98%)	280 (99%)	4 (1%)	59	29
1	DDD	272/291 (94%)	268 (98%)	4 (2%)	57	27
All	All	1110/1164 (95%)	1097 (99%)	13 (1%)	65	34

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	20[A]	ARG
1	AAA	20[B]	ARG
1	AAA	141	ARG
1	AAA	325	TRP
1	BBB	317	VAL
1	CCC	6	ASP
1	CCC	91	LEU
1	CCC	163	GLN
1	CCC	317	VAL
1	DDD	51[A]	LYS
1	DDD	51[B]	LYS
1	DDD	106	VAL
1	DDD	163	GLN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 17 are monoatomic - leaving 34 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	$\# Z > 2$
7	U78	BBB	406	-	13,13,13	0.30	0	16,16,16	0.32	0
3	EDO	DDD	408	-	3,3,3	0.05	0	2,2,2	0.17	0
3	EDO	DDD	405	-	3,3,3	0.17	0	2,2,2	0.04	0
3	EDO	AAA	402	-	3,3,3	0.16	0	2,2,2	0.23	0
11	OXE	DDD	410[A]	-	8,8,8	0.27	0	10,10,10	0.32	0
3	EDO	CCC	405[A]	-	3,3,3	0.08	0	2,2,2	0.15	0
3	EDO	CCC	404	4	3,3,3	0.05	0	2,2,2	0.26	0
3	EDO	DDD	407	-	3,3,3	0.05	0	2,2,2	0.09	0
6	GOL	CCC	409[A]	-	5,5,5	0.06	0	5,5,5	0.27	0
3	EDO	AAA	407	-	3,3,3	0.11	0	2,2,2	0.15	0
9	PG0	DDD	404	-	7,7,7	0.22	0	6,6,6	0.10	0
10	PGE	DDD	409	-	9,9,9	0.16	0	8,8,8	0.11	0
2	PLP	BBB	401	1	15,15,16	0.78	1 (6%)	21,22,23	0.95	2 (9%)
2	PLP	AAA	401[A]	1	15,15,16	0.86	1 (6%)	21,22,23	1.00	2 (9%)
3	EDO	AAA	408[A]	-	3,3,3	0.03	0	2,2,2	0.06	0
6	GOL	DDD	411[A]	-	5,5,5	0.08	0	5,5,5	0.40	0
3	EDO	CCC	405[B]	-	3,3,3	0.07	0	2,2,2	0.20	0
3	EDO	DDD	406	-	3,3,3	0.12	0	2,2,2	0.29	0
3	EDO	AAA	406[A]	-	3,3,3	0.11	0	2,2,2	0.11	0
3	EDO	AAA	409	-	3,3,3	0.06	0	2,2,2	0.16	0
6	GOL	CCC	409[B]	-	5,5,5	0.08	0	5,5,5	0.29	0
6	GOL	AAA	413[A]	-	5,5,5	0.06	0	5,5,5	0.28	0
3	EDO	AAA	406[B]	-	3,3,3	0.05	0	2,2,2	0.09	0
3	EDO	BBB	402	-	3,3,3	0.04	0	2,2,2	0.11	0
6	GOL	AAA	410	-	5,5,5	0.07	0	5,5,5	0.30	0
6	GOL	CCC	407	-	5,5,5	0.08	0	5,5,5	0.37	0
2	PLP	AAA	401[B]	1	15,15,16	0.80	1 (6%)	21,22,23	0.96	1 (4%)
2	PLP	CCC	401	1	15,15,16	0.78	1 (6%)	21,22,23	1.12	2 (9%)
2	PLP	DDD	401	1	15,15,16	0.75	1 (6%)	21,22,23	0.96	1 (4%)
6	GOL	CCC	402	-	5,5,5	0.09	0	5,5,5	0.31	0
7	U78	AAA	412	-	13,13,13	0.30	0	16,16,16	0.30	0
3	EDO	CCC	406	-	3,3,3	0.04	0	2,2,2	0.02	0
6	GOL	DDD	411[B]	-	5,5,5	0.11	0	5,5,5	0.29	0
3	EDO	CCC	408	-	3,3,3	0.03	0	2,2,2	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
7	U78	BBB	406	-	-	0/6/6/6	0/1/1/1
3	EDO	DDD	408	-	-	1/1/1/1	-
3	EDO	DDD	405	-	-	1/1/1/1	-
3	EDO	AAA	402	-	-	1/1/1/1	-
11	OXE	DDD	410[A]	-	-	-	0/1/1/1
3	EDO	CCC	405[A]	-	-	0/1/1/1	-
3	EDO	CCC	404	4	-	1/1/1/1	-
3	EDO	DDD	407	-	-	1/1/1/1	-
6	GOL	CCC	409[A]	-	-	2/4/4/4	-
3	EDO	AAA	407	-	-	1/1/1/1	-
9	PG0	DDD	404	-	-	2/5/5/5	-
10	PGE	DDD	409	-	-	4/7/7/7	-
2	PLP	BBB	401	1	-	0/6/6/8	0/1/1/1
2	PLP	AAA	401[A]	1	-	1/6/6/8	0/1/1/1
3	EDO	AAA	408[A]	-	-	1/1/1/1	-
6	GOL	DDD	411[A]	-	-	2/4/4/4	-
3	EDO	CCC	405[B]	-	-	1/1/1/1	-
3	EDO	DDD	406	-	-	0/1/1/1	-
3	EDO	AAA	406[A]	-	-	0/1/1/1	-
3	EDO	AAA	409	-	-	1/1/1/1	-
6	GOL	CCC	409[B]	-	-	4/4/4/4	-
6	GOL	AAA	413[A]	-	-	0/4/4/4	-
3	EDO	AAA	406[B]	-	-	1/1/1/1	-
3	EDO	BBB	402	-	-	1/1/1/1	-
6	GOL	AAA	410	-	-	2/4/4/4	-
6	GOL	CCC	407	-	-	4/4/4/4	-
2	PLP	AAA	401[B]	1	-	0/6/6/8	0/1/1/1
2	PLP	CCC	401	1	-	0/6/6/8	0/1/1/1
2	PLP	DDD	401	1	-	0/6/6/8	0/1/1/1
6	GOL	CCC	402	-	-	2/4/4/4	-
7	U78	AAA	412	-	-	0/6/6/6	0/1/1/1
3	EDO	CCC	406	-	-	0/1/1/1	-
6	GOL	DDD	411[B]	-	-	4/4/4/4	-
3	EDO	CCC	408	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401[A]	PLP	C4A-C4	-2.72	1.46	1.51
2	AAA	401[B]	PLP	C4A-C4	-2.48	1.46	1.51
2	DDD	401	PLP	C4A-C4	-2.47	1.46	1.51
2	BBB	401	PLP	C4A-C4	-2.37	1.46	1.51
2	CCC	401	PLP	C4A-C4	-2.24	1.47	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	401	PLP	O4P-C5A-C5	3.27	115.49	109.36
2	CCC	401	PLP	C4A-C4-C5	3.11	124.14	120.94
2	AAA	401[B]	PLP	O4P-C5A-C5	2.93	114.86	109.36
2	AAA	401[A]	PLP	O4P-C5A-C5	2.90	114.78	109.36
2	CCC	401	PLP	O4P-C5A-C5	2.43	113.92	109.36
2	BBB	401	PLP	O4P-C5A-C5	2.27	113.61	109.36
2	AAA	401[A]	PLP	C4A-C4-C5	2.17	123.17	120.94
2	BBB	401	PLP	C4A-C4-C5	2.03	123.03	120.94

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	410	GOL	C1-C2-C3-O3
6	CCC	402	GOL	O1-C1-C2-C3
6	CCC	407	GOL	C1-C2-C3-O3
6	CCC	409[A]	GOL	O2-C2-C3-O3
6	CCC	409[B]	GOL	O2-C2-C3-O3
6	CCC	407	GOL	O1-C1-C2-C3
6	CCC	409[A]	GOL	C1-C2-C3-O3
6	CCC	409[B]	GOL	C1-C2-C3-O3
6	DDD	411[A]	GOL	C1-C2-C3-O3
6	DDD	411[B]	GOL	O1-C1-C2-C3
6	DDD	411[B]	GOL	C1-C2-C3-O3
6	CCC	407	GOL	O2-C2-C3-O3
3	AAA	402	EDO	O1-C1-C2-O2
10	DDD	409	PGE	O3-C5-C6-O4
6	CCC	402	GOL	O1-C1-C2-O2
6	CCC	407	GOL	O1-C1-C2-O2
3	CCC	404	EDO	O1-C1-C2-O2
3	DDD	405	EDO	O1-C1-C2-O2
6	AAA	410	GOL	O2-C2-C3-O3
6	DDD	411[B]	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	AAA	401[A]	PLP	C6-C5-C5A-O4P
6	DDD	411[B]	GOL	O1-C1-C2-O2
10	DDD	409	PGE	C6-C5-O3-C4
6	DDD	411[A]	GOL	O2-C2-C3-O3
6	CCC	409[B]	GOL	O1-C1-C2-C3
3	DDD	407	EDO	O1-C1-C2-O2
3	AAA	406[B]	EDO	O1-C1-C2-O2
3	DDD	408	EDO	O1-C1-C2-O2
6	CCC	409[B]	GOL	O1-C1-C2-O2
10	DDD	409	PGE	C1-C2-O2-C3
3	AAA	407	EDO	O1-C1-C2-O2
3	CCC	405[B]	EDO	O1-C1-C2-O2
3	AAA	409	EDO	O1-C1-C2-O2
3	BBB	402	EDO	O1-C1-C2-O2
9	DDD	404	PG0	O1-C3-C4-O2
9	DDD	404	PG0	OTT-C1-C2-O1
10	DDD	409	PGE	O2-C3-C4-O3
3	AAA	408[A]	EDO	O1-C1-C2-O2
3	CCC	408	EDO	O1-C1-C2-O2

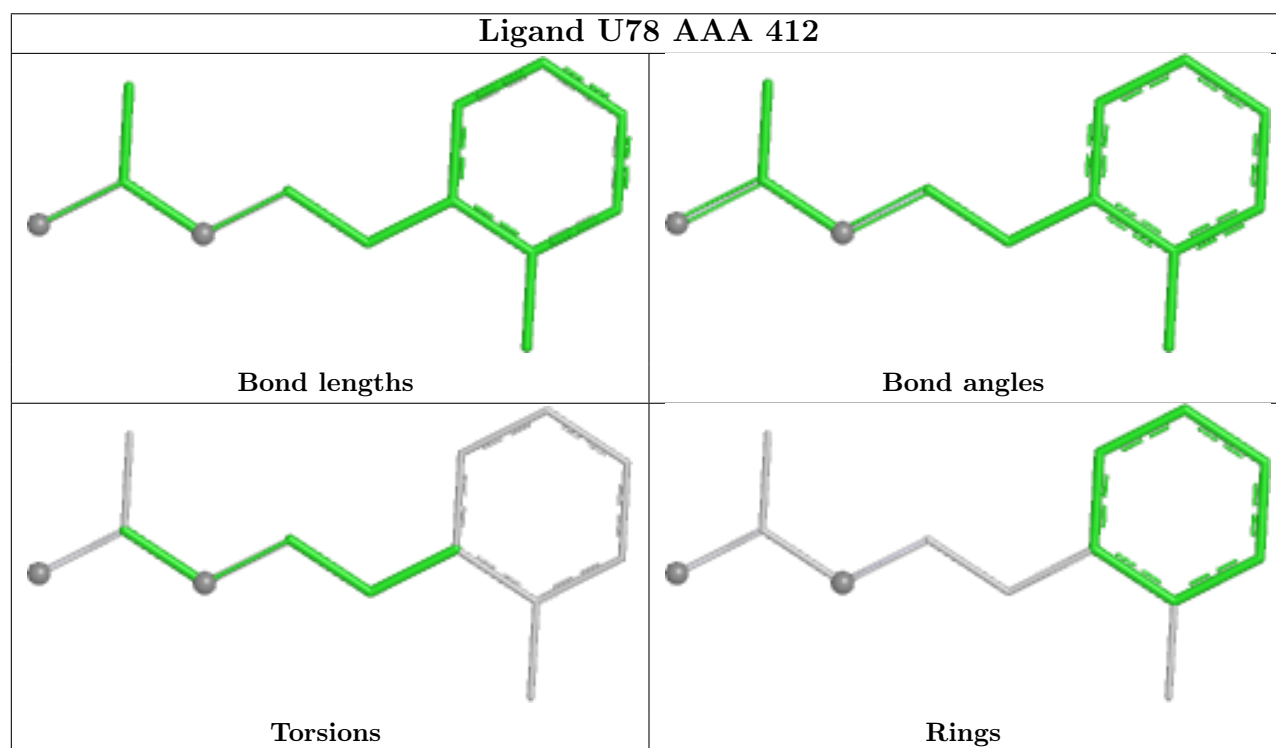
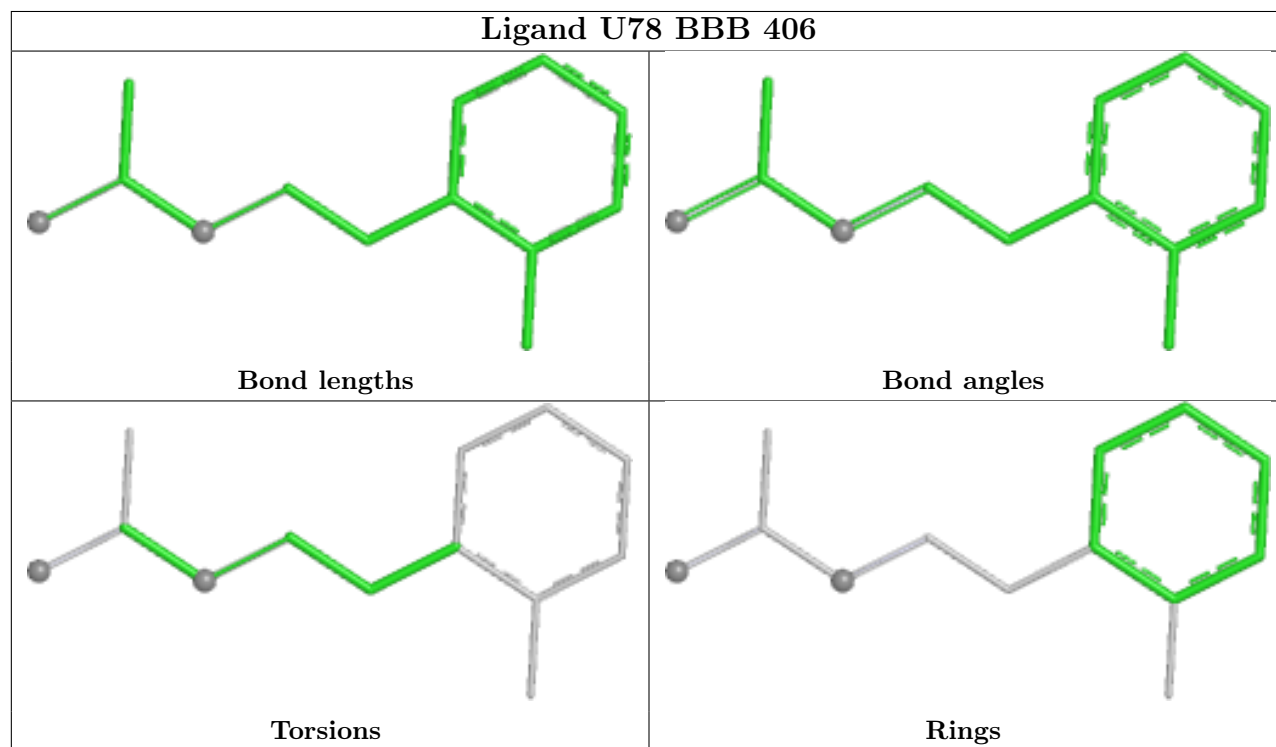
There are no ring outliers.

12 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CCC	404	EDO	2	0
6	CCC	409[A]	GOL	1	0
9	DDD	404	PG0	1	0
10	DDD	409	PGE	3	0
2	AAA	401[A]	PLP	1	0
6	DDD	411[A]	GOL	6	0
3	AAA	406[A]	EDO	1	0
6	AAA	413[A]	GOL	7	0
6	AAA	410	GOL	2	0
2	CCC	401	PLP	1	0
6	CCC	402	GOL	5	0
6	DDD	411[B]	GOL	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 ⓘ

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	AAA	322/346 (93%)	0.29	27 (8%) 17 21	7, 19, 45, 104	36 (11%)
1	BBB	307/346 (88%)	0.62	41 (13%) 7 9	11, 25, 51, 80	20 (6%)
1	CCC	317/346 (91%)	0.44	15 (4%) 36 44	7, 23, 45, 62	33 (10%)
1	DDD	310/346 (89%)	0.35	34 (10%) 10 14	9, 21, 43, 72	39 (12%)
All	All	1256/1384 (90%)	0.42	117 (9%) 14 19	7, 22, 48, 104	128 (10%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	231[A]	TYR	11.9
1	AAA	323	ILE	6.5
1	AAA	325	TRP	5.9
1	DDD	111[A]	PRO	5.6
1	AAA	319	LEU	5.1
1	CCC	113	CYS	4.7
1	DDD	68[A]	VAL	4.7
1	CCC	110	ALA	4.7
1	DDD	121[A]	TYR	4.5
1	AAA	320	THR	4.4
1	BBB	67	LEU	4.4
1	BBB	106	VAL	4.4
1	BBB	127	TYR	4.4
1	AAA	137	ASN	4.4
1	BBB	105	VAL	4.3
1	BBB	126	VAL	4.3
1	CCC	319	LEU	4.3
1	DDD	113[A]	CYS	4.2
1	AAA	322	SER	4.0
1	BBB	319	LEU	4.0
1	DDD	117[A]	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	DDD	116[A]	LEU	3.9
1	BBB	109	THR	3.8
1	BBB	320	THR	3.8
1	DDD	118[A]	ILE	3.7
1	DDD	114[A]	LYS	3.7
1	DDD	231	TYR	3.7
1	DDD	125	ILE	3.7
1	BBB	125	ILE	3.6
1	CCC	111	PRO	3.5
1	DDD	67[A]	LEU	3.5
1	CCC	72	LEU	3.4
1	AAA	131[A]	SER	3.4
1	DDD	130	PRO	3.4
1	BBB	121	TYR	3.3
1	BBB	104	ILE	3.3
1	DDD	318	ASP	3.2
1	CCC	3[A]	ALA	3.2
1	DDD	120[A]	ALA	3.1
1	AAA	134	SER	3.0
1	AAA	324	THR	3.0
1	DDD	109[A]	THR	3.0
1	CCC	116	LEU	3.0
1	CCC	117	ALA	2.9
1	BBB	100	ILE	2.9
1	DDD	106	VAL	2.9
1	DDD	126[A]	VAL	2.9
1	BBB	230	LEU	2.9
1	CCC	33[A]	ILE	2.8
1	BBB	231[A]	TYR	2.8
1	DDD	122[A]	GLY	2.8
1	BBB	149	ILE	2.8
1	AAA	121	TYR	2.8
1	DDD	317	VAL	2.8
1	CCC	108[A]	GLN	2.7
1	BBB	82	HIS	2.7
1	BBB	83	SER	2.7
1	DDD	4[A]	GLN	2.7
1	BBB	138	VAL	2.7
1	AAA	321	SER	2.7
1	BBB	123	ALA	2.6
1	DDD	127	TYR	2.6
1	BBB	124	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	BBB	130	PRO	2.6
1	AAA	133	GLU	2.6
1	BBB	107	PRO	2.6
1	DDD	104	ILE	2.6
1	BBB	137	ASN	2.6
1	DDD	138	VAL	2.6
1	BBB	139	ALA	2.5
1	CCC	109	THR	2.5
1	BBB	133	GLU	2.5
1	AAA	116	LEU	2.5
1	BBB	116	LEU	2.5
1	AAA	130	PRO	2.5
1	AAA	317	VAL	2.5
1	AAA	113	CYS	2.5
1	AAA	120	ALA	2.5
1	BBB	148	GLY	2.5
1	DDD	66	SER	2.4
1	AAA	138	VAL	2.4
1	BBB	102	ALA	2.4
1	DDD	108[A]	GLN	2.4
1	AAA	135[A]	ARG	2.4
1	DDD	110[A]	ALA	2.4
1	DDD	128[A]	CYS	2.4
1	AAA	149	ILE	2.4
1	DDD	134	SER	2.4
1	BBB	103	TYR	2.3
1	AAA	318	ASP	2.3
1	BBB	108	GLN	2.3
1	BBB	113	CYS	2.3
1	BBB	79	VAL	2.3
1	CCC	317	VAL	2.3
1	BBB	135	ARG	2.3
1	DDD	82[A]	HIS	2.3
1	BBB	33	ILE	2.3
1	BBB	66	SER	2.2
1	BBB	4	GLN	2.2
1	BBB	128	CYS	2.2
1	DDD	34[A]	LEU	2.2
1	DDD	107	PRO	2.2
1	AAA	141	ARG	2.2
1	CCC	34	LEU	2.1
1	BBB	80	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	110	ALA	2.1
1	AAA	140	LYS	2.1
1	DDD	75	LYS	2.1
1	BBB	136	GLU	2.1
1	AAA	109	THR	2.0
1	AAA	68	VAL	2.0
1	CCC	293[A]	VAL	2.0
1	DDD	131	SER	2.0
1	DDD	112[A]	ASP	2.0
1	AAA	148	GLY	2.0
1	BBB	120	ALA	2.0
1	BBB	64	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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, 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
8	MG	BBB	407	1/1	0.65	0.31	79,79,79,79	0
6	GOL	DDD	411[B]	6/6	0.74	0.21	16,18,18,18	6
6	GOL	DDD	411[A]	6/6	0.74	0.21	42,43,44,44	6
10	PGE	DDD	409	10/10	0.75	0.21	57,60,62,63	0
3	EDO	DDD	407	4/4	0.79	0.17	57,58,59,61	0
6	GOL	AAA	410	6/6	0.79	0.16	46,47,51,53	0
3	EDO	CCC	408	4/4	0.79	0.18	48,50,51,53	0
3	EDO	CCC	406	4/4	0.80	0.15	46,46,48,51	0
3	EDO	AAA	406[A]	4/4	0.80	0.16	35,40,42,42	4
3	EDO	DDD	406	4/4	0.80	0.15	36,40,43,45	0
3	EDO	AAA	406[B]	4/4	0.80	0.16	27,29,29,30	4

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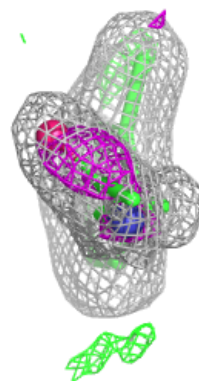
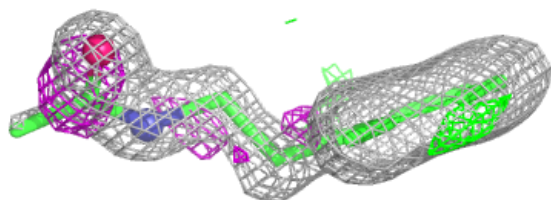
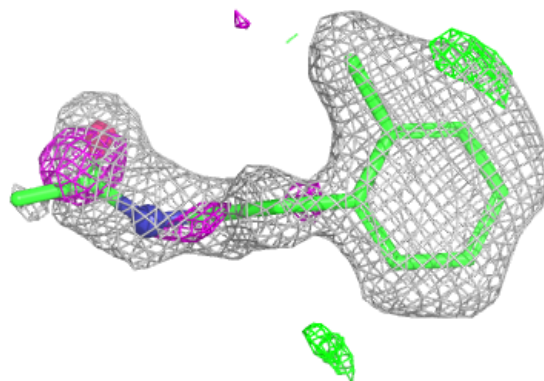
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	BBB	405	1/1	0.80	0.17	53,53,53,53	0
3	EDO	AAA	409	4/4	0.81	0.18	62,63,63,66	0
6	GOL	AAA	413[A]	6/6	0.81	0.18	25,27,27,29	6
3	EDO	CCC	404	4/4	0.82	0.15	51,51,52,57	0
4	NA	AAA	414[A]	1/1	0.82	0.24	80,80,80,80	1
4	NA	AAA	414[B]	1/1	0.82	0.24	46,46,46,46	1
6	GOL	CCC	407	6/6	0.82	0.16	54,55,56,59	0
9	PG0	DDD	404	8/8	0.83	0.18	28,47,49,50	0
6	GOL	CCC	402	6/6	0.83	0.17	43,45,47,47	0
7	U78	AAA	412	13/13	0.84	0.14	26,29,40,40	0
3	EDO	BBB	402	4/4	0.84	0.16	50,53,55,56	0
3	EDO	AAA	407	4/4	0.84	0.15	35,37,38,40	0
3	EDO	AAA	402	4/4	0.84	0.16	40,42,43,46	0
6	GOL	CCC	409[B]	6/6	0.85	0.15	52,53,53,53	6
6	GOL	CCC	409[A]	6/6	0.85	0.15	36,37,37,38	6
7	U78	BBB	406	13/13	0.85	0.14	34,35,44,47	0
3	EDO	AAA	408[A]	4/4	0.87	0.19	40,40,40,41	4
8	MG	DDD	412	1/1	0.87	0.12	49,49,49,49	0
3	EDO	DDD	408	4/4	0.88	0.14	47,47,48,48	0
3	EDO	DDD	405	4/4	0.88	0.14	36,38,43,47	0
11	OXE	DDD	410[A]	8/8	0.88	0.12	22,23,23,24	8
4	NA	CCC	411	1/1	0.89	0.15	57,57,57,57	0
3	EDO	CCC	405[B]	4/4	0.90	0.11	30,31,31,31	4
4	NA	AAA	403	1/1	0.90	0.09	60,60,60,60	0
3	EDO	CCC	405[A]	4/4	0.90	0.11	35,36,37,37	4
4	NA	CCC	410	1/1	0.91	0.12	59,59,59,59	0
4	NA	DDD	402	1/1	0.94	0.15	33,33,33,33	0
2	PLP	CCC	401	15/16	0.98	0.05	17,17,19,20	0
2	PLP	DDD	401	15/16	0.98	0.05	15,15,17,17	0
2	PLP	AAA	401[A]	15/16	0.98	0.05	13,14,15,15	15
4	NA	AAA	405	1/1	0.98	0.04	28,28,28,28	0
2	PLP	AAA	401[B]	15/16	0.98	0.05	13,14,16,16	15
5	CA	DDD	403	1/1	0.99	0.04	17,17,17,17	0
4	NA	AAA	411	1/1	0.99	0.04	22,22,22,22	0
4	NA	BBB	404	1/1	0.99	0.06	20,20,20,20	0
2	PLP	BBB	401	15/16	0.99	0.04	18,19,21,21	0
5	CA	AAA	404	1/1	0.99	0.02	15,15,15,15	0
5	CA	BBB	403	1/1	0.99	0.04	24,24,24,24	0
5	CA	CCC	403[A]	1/1	0.99	0.03	17,17,17,17	1
5	CA	CCC	403[B]	1/1	0.99	0.03	20,20,20,20	1

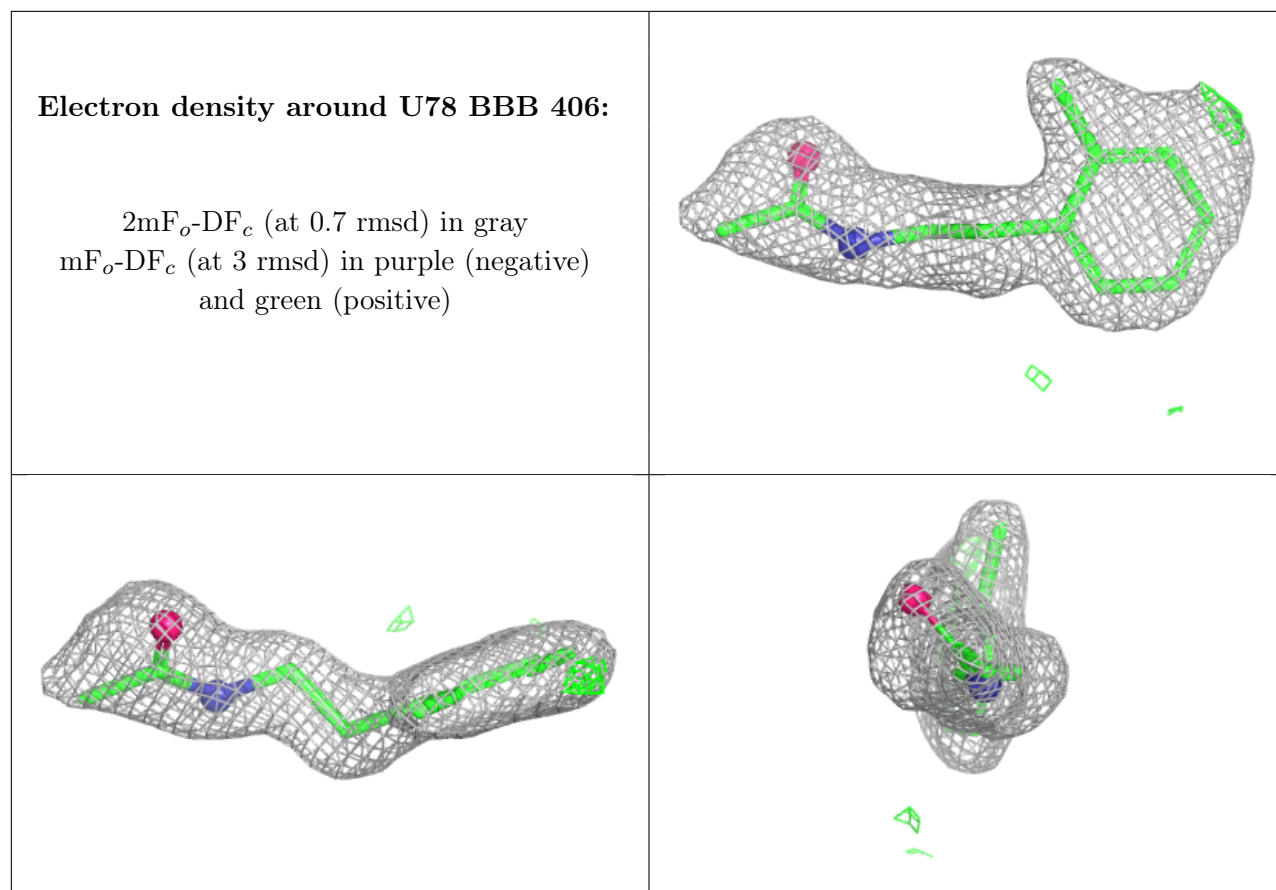
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around U78 AAA 412:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.