



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:35 AM UTC

PDB ID : 7NBC / pdb_00007nbc
Title : Crystal structure of human serine racemase in complex with DSiP fragment
Z2856434779, XChem fragment screen.
Authors : Koulouris, C.R.; Roe, S.M.
Deposited on : 2021-01-26
Resolution : 1.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

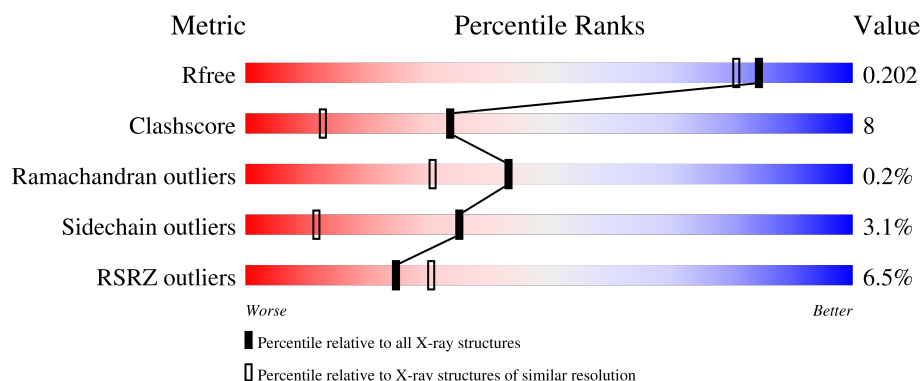
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	3% 79% 12% • 7%
1	BBB	346	12% 74% 14% • 10%
1	CCC	346	3% 84% 9% • 6%
1	DDD	346	6% 83% 8% 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
3	GOL	AAA	403	-	-	X	-
3	GOL	AAA	409	-	-	X	-
3	GOL	BBB	405	-	-	X	-
6	EDO	DDD	406	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11179 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	323	Total	C	N	O	S	0	28	0
			2651	1678	446	515	12			
1	BBB	313	Total	C	N	O	S	0	17	0
			2410	1534	400	465	11			
1	CCC	324	Total	C	N	O	S	0	19	1
			2545	1623	424	486	12			
1	DDD	317	Total	C	N	O	S	0	19	0
			2509	1594	427	475	13			

There are 32 discrepancies between the modelled and reference sequences:

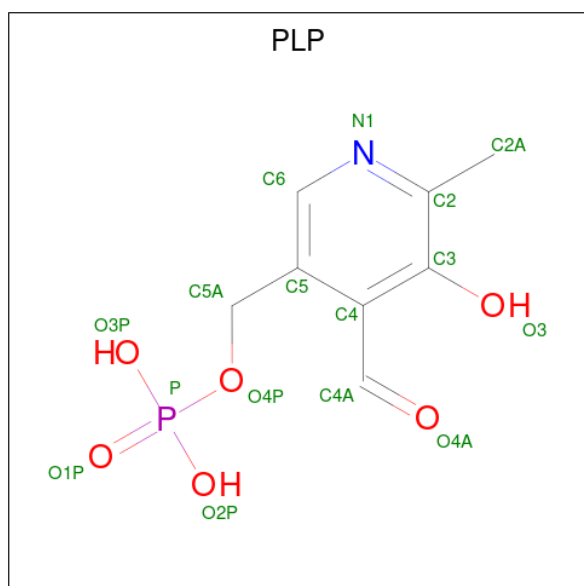
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	6	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	341	HIS	-	expression tag	UNP Q9GZT4
AAA	342	HIS	-	expression tag	UNP Q9GZT4
AAA	343	HIS	-	expression tag	UNP Q9GZT4
AAA	344	HIS	-	expression tag	UNP Q9GZT4
AAA	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	0
			15	8	1	5	1		
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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total	Ca	0	0
			2	2		
4	BBB	2	Total	Ca	0	0
			2	2		

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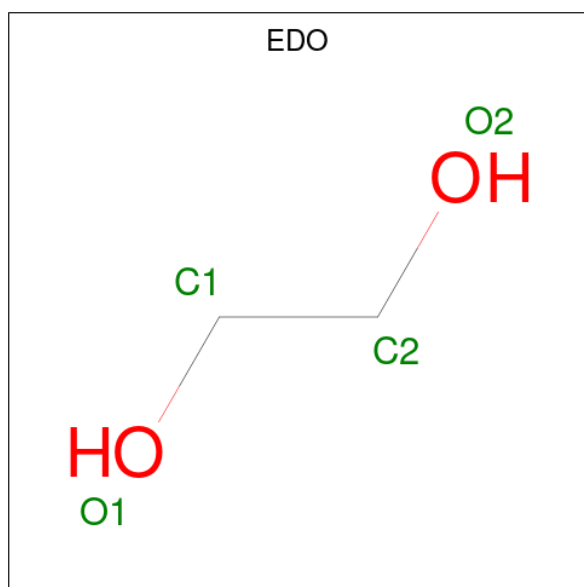
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	CCC	1	Total	Ca	0	1
			2	2		
4	DDD	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Mg	0	0
			1	1		
5	DDD	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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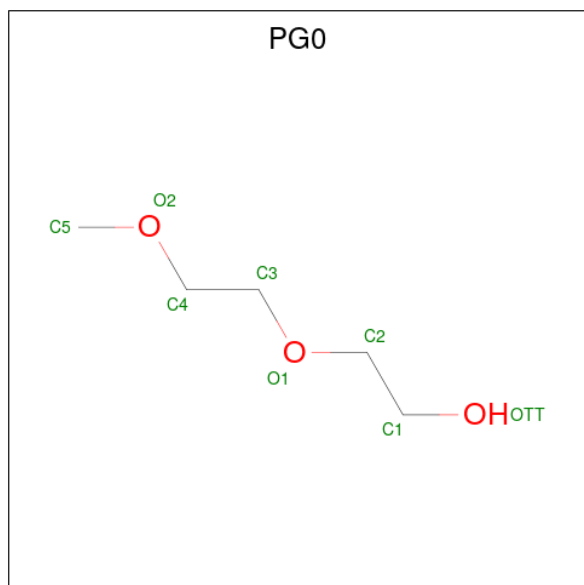
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	CCC	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	3	Total	Na	0	0
			3	3		
7	DDD	1	Total	Na	0	0
			1	1		

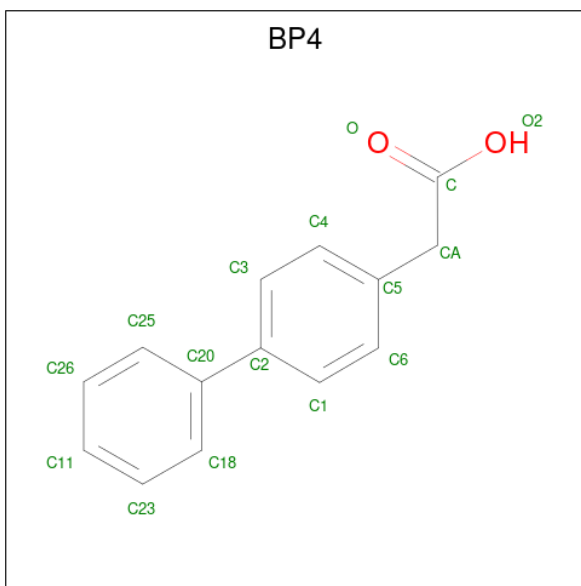
- Molecule 8 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



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

- Molecule 9 is biphenyl-4-ylacetic acid (CCD ID: BP4) (formula: C₁₄H₁₂O₂) (labeled as "Lig-

and of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	CCC	1	Total	C	O	0	0
			16	14	2		

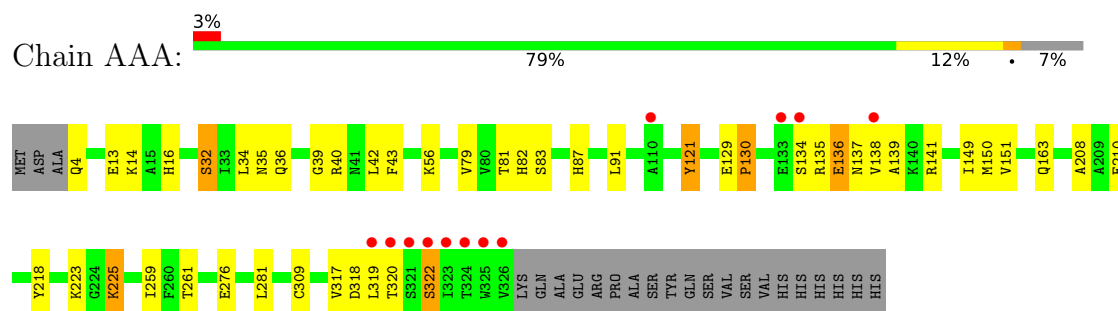
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	262	Total	O	0	0
			262	262		
10	BBB	154	Total	O	0	1
			154	154		
10	CCC	217	Total	O	0	0
			217	217		
10	DDD	234	Total	O	0	0
			234	234		

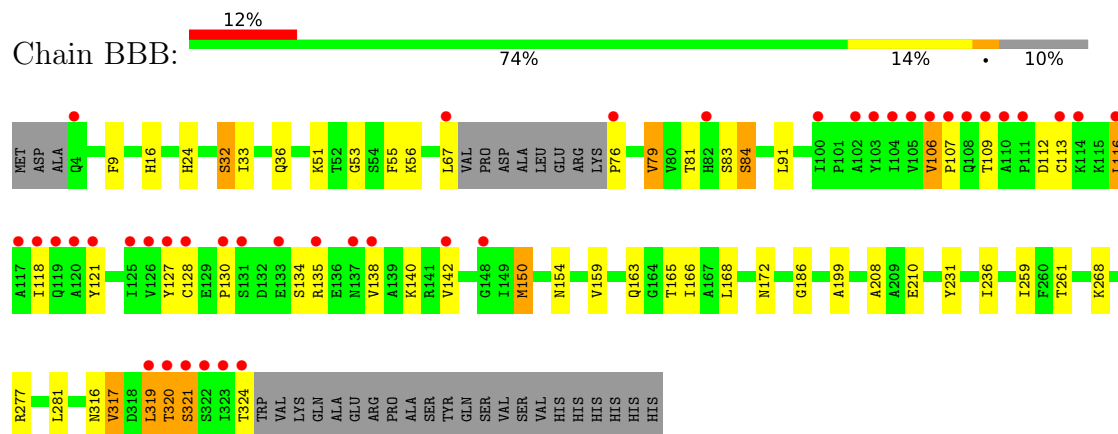
3 Residue-property plots [i](#)

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.

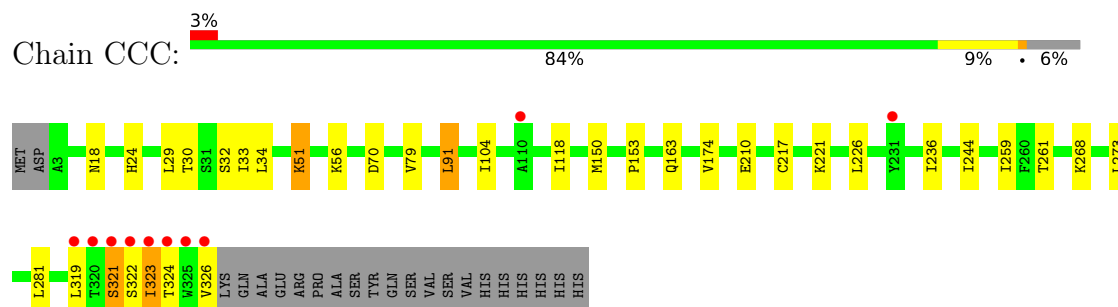
• Molecule 1: Serine racemase



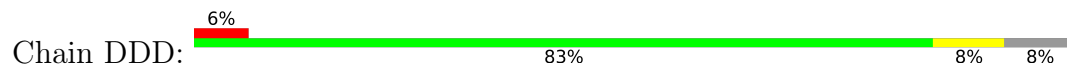
• Molecule 1: Serine racemase

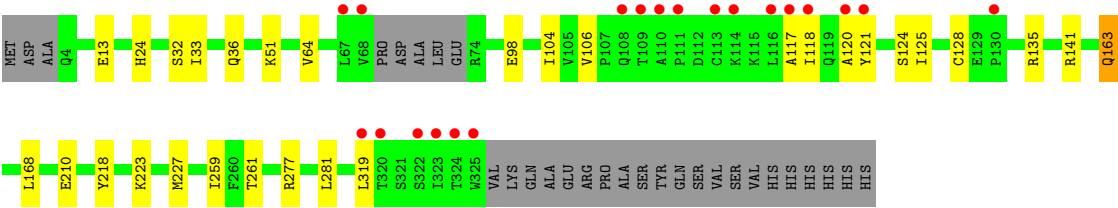


• Molecule 1: Serine racemase



• 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	48.15Å 154.86Å 85.48Å 90.00° 98.08° 90.00°	Depositor
Resolution (Å)	77.40 – 1.71 77.40 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.1 (77.40-1.71) 98.1 (77.40-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.174 , 0.202 0.174 , 0.202	Depositor DCC
R_{free} test set	6527 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11179	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CA, BP4, NA, PLP, MG, GOL, PG0

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	0.57	0/2697	0.91	3/3676 (0.1%)
1	BBB	0.53	0/2452	0.93	0/3352
1	CCC	0.52	0/2591	0.90	0/3542
1	DDD	0.54	0/2552	0.94	2/3480 (0.1%)
All	All	0.54	0/10292	0.92	5/14050 (0.0%)

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	BBB	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	121	TYR	CB-CA-C	7.42	123.37	110.01
1	DDD	163	GLN	CB-CG-CD	6.04	122.87	112.60
1	AAA	130	PRO	N-CD-CG	-6.00	94.19	103.20
1	AAA	276	GLU	CB-CG-CD	5.20	121.44	112.60
1	DDD	121	TYR	CB-CA-C	5.11	120.11	109.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	319	LEU	Peptide

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	AAA	2651	0	2653	46	0
1	BBB	2410	0	2364	46	0
1	CCC	2545	0	2539	36	0
1	DDD	2509	0	2512	29	0
2	AAA	15	0	6	1	0
2	BBB	15	0	6	1	0
2	CCC	15	0	6	1	0
2	DDD	15	0	6	0	0
3	AAA	30	0	39	14	0
3	BBB	18	0	24	5	0
3	CCC	12	0	16	6	0
4	AAA	2	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	DDD	1	0	0	0	0
6	AAA	8	0	11	0	0
6	BBB	8	0	12	2	0
6	CCC	8	0	12	3	0
6	DDD	16	0	24	5	0
7	AAA	3	0	0	0	0
7	DDD	1	0	0	0	0
8	CCC	8	0	12	5	0
9	CCC	16	0	11	1	0
10	AAA	262	0	0	6	0
10	BBB	154	0	0	3	0
10	CCC	217	0	0	6	0
10	DDD	234	0	0	3	1
All	All	11179	0	10253	160	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.

The worst 5 of 160 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:AAA:14[B]:LYS:HE3	10:AAA:517:HOH:O	1.66	0.94
1:DDD:223:LYS:HG2	10:DDD:505:HOH:O	1.68	0.93
1:DDD:261:THR:H	6:DDD:406:EDO:H12	1.36	0.90
1:AAA:149:ILE:HA	3:AAA:403:GOL:H32	1.60	0.84
1:CCC:34[A]:LEU:HD21	1:CCC:273[A]:LEU:CD2	2.09	0.83

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)
10:DDD:549:HOH:O	10:DDD:661:HOH:O[1_455]	1.84	0.36

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	349/346 (101%)	337 (97%)	12 (3%)	0	100	100
1	BBB	325/346 (94%)	313 (96%)	11 (3%)	1 (0%)	36	24
1	CCC	341/346 (99%)	330 (97%)	10 (3%)	1 (0%)	36	24
1	DDD	332/346 (96%)	318 (96%)	14 (4%)	0	100	100
All	All	1347/1384 (97%)	1298 (96%)	47 (4%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	319	LEU
1	CCC	321	SER

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	293/291 (101%)	284 (97%)	9 (3%)	35	12
1	BBB	256/291 (88%)	244 (95%)	12 (5%)	23	4
1	CCC	275/291 (94%)	267 (97%)	8 (3%)	37	14
1	DDD	272/291 (94%)	269 (99%)	3 (1%)	65	50
All	All	1096/1164 (94%)	1064 (97%)	32 (3%)	35	14

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	326	VAL
1	DDD	124	SER
1	BBB	84	SER
1	BBB	79	VAL
1	DDD	141	ARG

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

Of 39 ligands modelled in this entry, 13 are monoatomic - leaving 26 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	GOL	BBB	407	-	5,5,5	0.10	0	5,5,5	0.35	0
2	PLP	DDD	401	1	15,15,16	0.74	1 (6%)	21,22,23	1.00	1 (4%)
6	EDO	AAA	408	4	3,3,3	0.29	0	2,2,2	0.33	0
3	GOL	AAA	410	5	5,5,5	0.12	0	5,5,5	0.42	0
3	GOL	AAA	402	-	5,5,5	0.08	0	5,5,5	0.39	0
6	EDO	AAA	407	-	3,3,3	0.19	0	2,2,2	0.20	0
3	GOL	BBB	405	-	5,5,5	0.10	0	5,5,5	0.16	0
3	GOL	AAA	403	-	5,5,5	0.09	0	5,5,5	0.34	0
6	EDO	DDD	407	-	3,3,3	0.05	0	2,2,2	0.25	0
3	GOL	AAA	409	-	5,5,5	0.10	0	5,5,5	0.49	0
3	GOL	AAA	406	-	5,5,5	0.17	0	5,5,5	0.25	0
6	EDO	DDD	408	-	3,3,3	0.14	0	2,2,2	0.37	0
6	EDO	BBB	408	-	3,3,3	0.26	0	2,2,2	0.43	0
6	EDO	CCC	407	-	3,3,3	0.23	0	2,2,2	0.22	0
3	GOL	CCC	408	-	5,5,5	0.10	0	5,5,5	0.36	0
2	PLP	CCC	401	1	15,15,16	0.84	1 (6%)	21,22,23	1.21	2 (9%)
3	GOL	BBB	402	-	5,5,5	0.09	0	5,5,5	0.30	0
6	EDO	CCC	406	-	3,3,3	0.21	0	2,2,2	0.25	0
9	BP4	CCC	405	-	17,17,17	0.62	1 (5%)	22,22,22	0.52	0
3	GOL	CCC	402	-	5,5,5	0.06	0	5,5,5	0.38	0
8	PG0	CCC	404	-	7,7,7	0.23	0	6,6,6	0.13	0
6	EDO	DDD	406	-	3,3,3	0.10	0	2,2,2	0.17	0
2	PLP	AAA	401	1	15,15,16	0.86	1 (6%)	21,22,23	1.05	1 (4%)
6	EDO	BBB	406	-	3,3,3	0.12	0	2,2,2	0.11	0
6	EDO	DDD	405	-	3,3,3	0.18	0	2,2,2	0.49	0
2	PLP	BBB	401	1	15,15,16	0.77	1 (6%)	21,22,23	1.03	1 (4%)

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	GOL	BBB	407	-	-	2/4/4/4	-
2	PLP	DDD	401	1	-	0/6/6/8	0/1/1/1
6	EDO	AAA	408	4	-	0/1/1/1	-
3	GOL	AAA	410	5	-	0/4/4/4	-
3	GOL	AAA	402	-	-	2/4/4/4	-
6	EDO	AAA	407	-	-	0/1/1/1	-
3	GOL	BBB	405	-	-	2/4/4/4	-
3	GOL	AAA	403	-	-	2/4/4/4	-
6	EDO	DDD	407	-	-	1/1/1/1	-
3	GOL	AAA	409	-	-	4/4/4/4	-
3	GOL	AAA	406	-	-	2/4/4/4	-
6	EDO	DDD	408	-	-	1/1/1/1	-
6	EDO	BBB	408	-	-	0/1/1/1	-
6	EDO	CCC	407	-	-	1/1/1/1	-
3	GOL	CCC	408	-	-	2/4/4/4	-
2	PLP	CCC	401	1	-	0/6/6/8	0/1/1/1
3	GOL	BBB	402	-	-	2/4/4/4	-
6	EDO	CCC	406	-	-	0/1/1/1	-
9	BP4	CCC	405	-	-	0/8/8/8	0/2/2/2
3	GOL	CCC	402	-	-	0/4/4/4	-
8	PG0	CCC	404	-	-	2/5/5/5	-
6	EDO	DDD	406	-	-	1/1/1/1	-
2	PLP	AAA	401	1	-	0/6/6/8	0/1/1/1
6	EDO	BBB	406	-	-	0/1/1/1	-
6	EDO	DDD	405	-	-	1/1/1/1	-
2	PLP	BBB	401	1	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401	PLP	C4A-C4	-2.94	1.45	1.51
2	CCC	401	PLP	C4A-C4	-2.52	1.46	1.51
2	DDD	401	PLP	C4A-C4	-2.44	1.46	1.51
9	CCC	405	BP4	O2-C	-2.35	1.23	1.30
2	BBB	401	PLP	C4A-C4	-2.35	1.46	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	401	PLP	C4A-C4-C5	3.40	124.44	120.94
2	AAA	401	PLP	O4P-C5A-C5	3.32	115.58	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	401	PLP	O4P-C5A-C5	3.27	115.48	109.36
2	CCC	401	PLP	O4P-C5A-C5	2.80	114.60	109.36
2	BBB	401	PLP	C4A-C4-C5	2.75	123.77	120.94

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	402	GOL	C1-C2-C3-O3
3	AAA	403	GOL	C1-C2-C3-O3
3	AAA	409	GOL	C1-C2-C3-O3
3	BBB	402	GOL	C1-C2-C3-O3
3	BBB	407	GOL	O1-C1-C2-C3

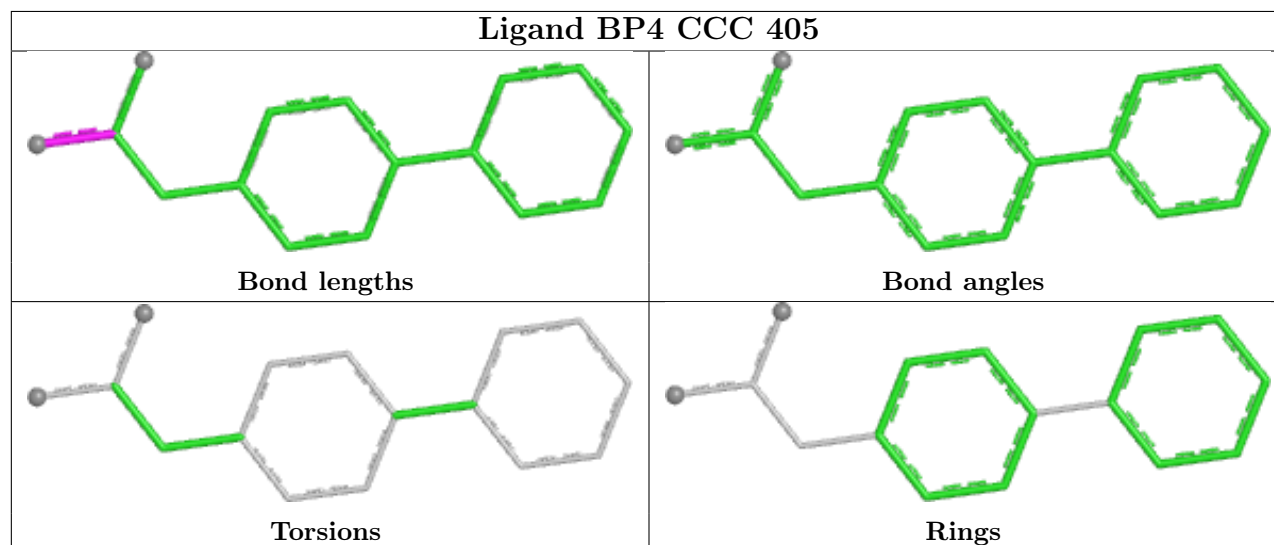
There are no ring outliers.

16 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	402	GOL	1	0
3	BBB	405	GOL	5	0
3	AAA	403	GOL	5	0
3	AAA	409	GOL	6	0
3	AAA	406	GOL	2	0
6	BBB	408	EDO	2	0
6	CCC	407	EDO	2	0
3	CCC	408	GOL	3	0
2	CCC	401	PLP	1	0
6	CCC	406	EDO	1	0
9	CCC	405	BP4	1	0
3	CCC	402	GOL	3	0
8	CCC	404	PG0	5	0
6	DDD	406	EDO	5	0
2	AAA	401	PLP	1	0
2	BBB	401	PLP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	323/346 (93%)	-0.12	12 (3%) 45 53	7, 21, 57, 135	28 (8%)
1	BBB	313/346 (90%)	0.42	41 (13%) 7 11	12, 29, 86, 132	17 (5%)
1	CCC	324/346 (93%)	-0.02	10 (3%) 51 61	10, 25, 53, 126	19 (5%)
1	DDD	317/346 (91%)	0.02	20 (6%) 26 31	11, 24, 74, 133	19 (5%)
All	All	1277/1384 (92%)	0.07	83 (6%) 25 30	7, 25, 72, 135	83 (6%)

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	326	VAL	6.0
1	DDD	325	TRP	5.6
1	BBB	106	VAL	5.3
1	AAA	323	ILE	5.2
1	CCC	319	LEU	5.2

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](#)

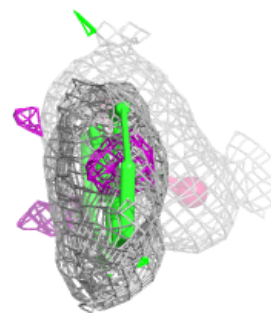
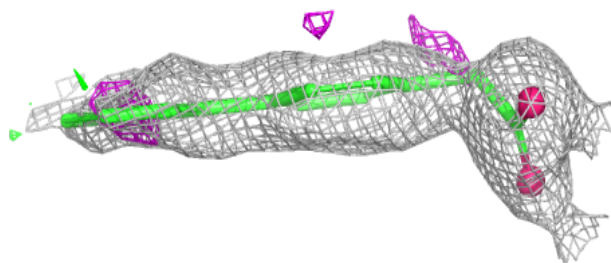
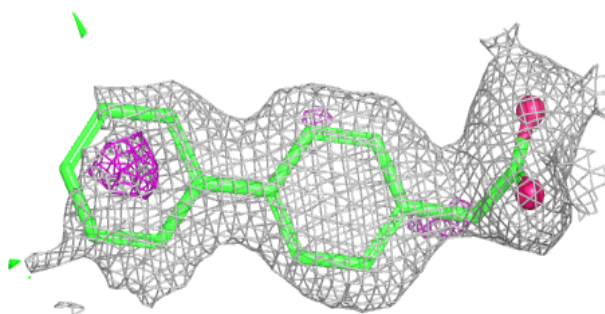
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	AAA	410	6/6	0.71	0.15	57,58,59,59	0
8	PG0	CCC	404	8/8	0.73	0.18	45,49,51,52	0
3	GOL	BBB	402	6/6	0.76	0.16	55,64,65,73	0
3	GOL	CCC	402	6/6	0.77	0.17	54,58,61,62	0
7	NA	DDD	404	1/1	0.79	0.11	56,56,56,56	0
3	GOL	BBB	407	6/6	0.79	0.17	69,72,76,76	0
3	GOL	AAA	403	6/6	0.80	0.17	35,42,46,48	0
6	EDO	BBB	406	4/4	0.80	0.14	43,45,47,51	0
6	EDO	AAA	408	4/4	0.82	0.14	35,42,49,50	0
3	GOL	BBB	405	6/6	0.82	0.17	50,53,56,59	0
7	NA	AAA	413	1/1	0.83	0.17	58,58,58,58	0
6	EDO	AAA	407	4/4	0.84	0.18	38,40,42,46	0
6	EDO	DDD	407	4/4	0.85	0.17	46,46,48,49	0
3	GOL	CCC	408	6/6	0.85	0.14	38,43,50,52	0
3	GOL	AAA	409	6/6	0.86	0.12	45,46,47,50	0
3	GOL	AAA	402	6/6	0.86	0.14	45,52,54,55	0
9	BP4	CCC	405	16/16	0.86	0.13	30,43,52,52	0
7	NA	AAA	414	1/1	0.87	0.14	61,61,61,61	0
6	EDO	DDD	408	4/4	0.88	0.12	49,50,52,53	0
6	EDO	CCC	407	4/4	0.90	0.11	36,36,41,51	0
6	EDO	DDD	405	4/4	0.90	0.12	30,32,36,45	0
6	EDO	CCC	406	4/4	0.90	0.12	35,38,41,44	0
3	GOL	AAA	406	6/6	0.91	0.13	28,34,42,54	0
6	EDO	BBB	408	4/4	0.91	0.12	32,38,39,41	0
6	EDO	DDD	406	4/4	0.92	0.11	34,36,37,38	0
7	NA	AAA	412	1/1	0.95	0.17	49,49,49,49	0
5	MG	DDD	403	1/1	0.95	0.08	39,39,39,39	0
5	MG	AAA	405	1/1	0.98	0.04	27,27,27,27	0
2	PLP	BBB	401	15/16	0.98	0.04	19,20,22,23	0
2	PLP	CCC	401	15/16	0.98	0.05	17,18,20,20	0
2	PLP	AAA	401	15/16	0.98	0.05	15,16,17,18	0
4	CA	AAA	411	1/1	0.98	0.10	30,30,30,30	0
4	CA	BBB	404	1/1	0.98	0.10	40,40,40,40	0
4	CA	BBB	403	1/1	0.99	0.03	27,27,27,27	0
2	PLP	DDD	401	15/16	0.99	0.04	16,17,19,19	0
4	CA	CCC	403[B]	1/1	1.00	0.02	30,30,30,30	1
4	CA	DDD	402	1/1	1.00	0.03	22,22,22,22	0
4	CA	AAA	404	1/1	1.00	0.02	18,18,18,18	0
4	CA	CCC	403[A]	1/1	1.00	0.02	13,13,13,13	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 BP4 CCC 405:

$2mF_o-DF_c$ (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.