



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2022 – 01:09 pm BST

PDB ID : 6ZUJ
Title : Human serine racemase holoenzyme from 20% DMSO soak (XChem crystallographic fragment screen).
Authors : Koulouris, C.R.; Bax, B.D.; Roe, S.M.; Atack, J.R.
Deposited on : 2020-07-23
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28

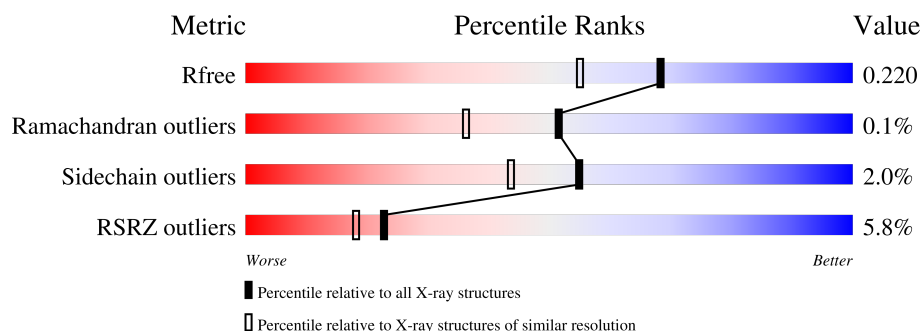
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>• 7%</div> </div> </div>
1	BBB	346	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>• 11%</div> </div> </div>
1	CCC	346	<div> <div>9%</div> <div> <div></div> <div>90%</div> <div>• 7%</div> </div> </div>
1	DDD	346	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10905 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	P	S	0	21	0
			2583	1640	432	499	1	11			
1	BBB	308	Total	C	N	O	P	S	0	17	0
			2386	1520	395	459	1	11			
1	CCC	323	Total	C	N	O	P	S	0	18	0
			2522	1607	417	486	1	11			
1	DDD	317	Total	C	N	O	P	S	0	15	0
			2484	1583	418	469	1	13			

There are 32 discrepancies between the modelled and reference sequences:

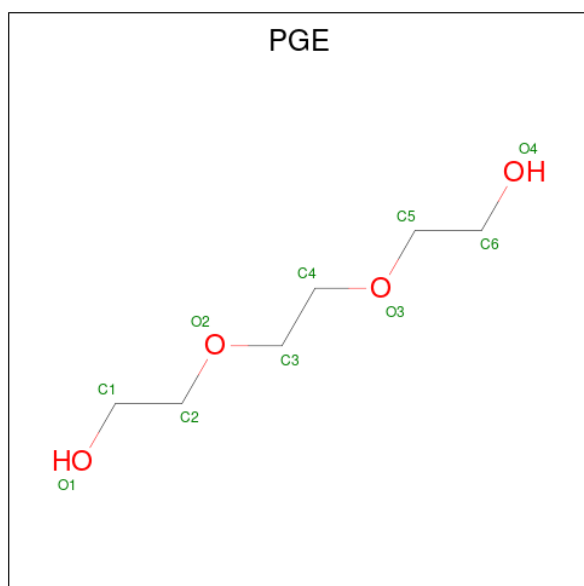
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	6	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	341	HIS	-	expression tag	UNP Q9GZT4
AAA	342	HIS	-	expression tag	UNP Q9GZT4
AAA	343	HIS	-	expression tag	UNP Q9GZT4
AAA	344	HIS	-	expression tag	UNP Q9GZT4
AAA	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 TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	CCC	1	Total	C	O	0	0
			5	3	2		
2	CCC	1	Total	C	O	0	0
			10	6	4		
2	DDD	1	Total	C	O	0	0
			8	5	3		
2	DDD	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Mg	0	0
			1	1		

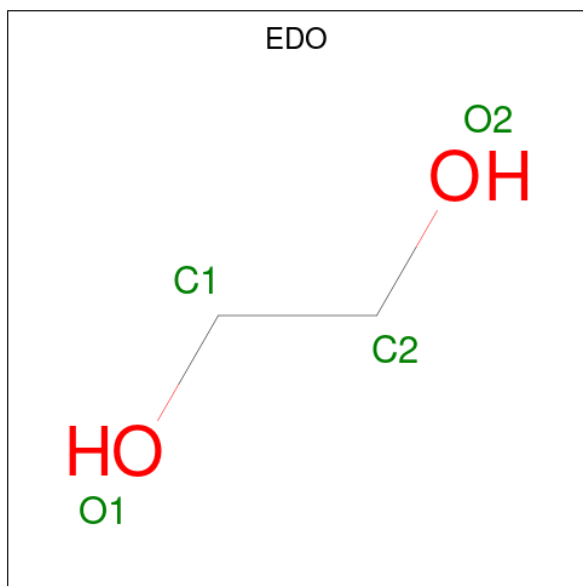
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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	0
			1	1		
5	DDD	1	Total	Ca	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	3	Total	Na	0	0
			3	3		
6	BBB	2	Total	Na	0	0
			2	2		
6	DDD	1	Total	Na	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



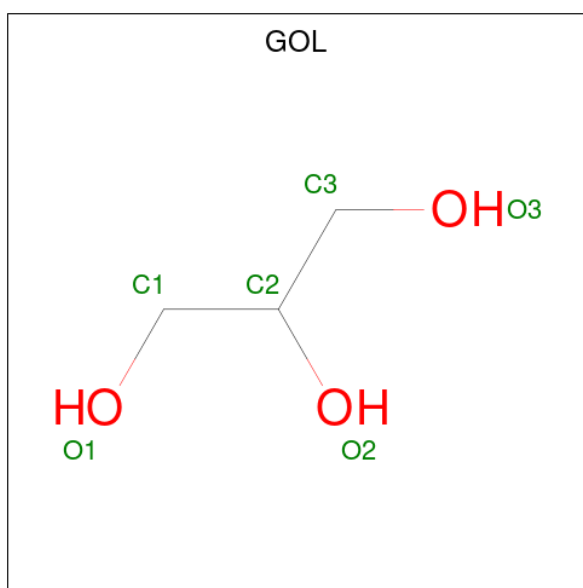
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	BBB	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4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

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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

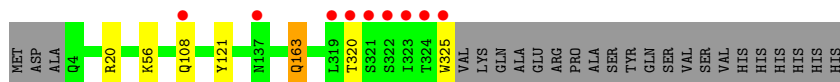
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	280	Total 280	O 280	0	0
9	BBB	101	Total 102	O 102	0	1
9	CCC	189	Total 190	O 190	0	1
9	DDD	222	Total 222	O 222	0	0

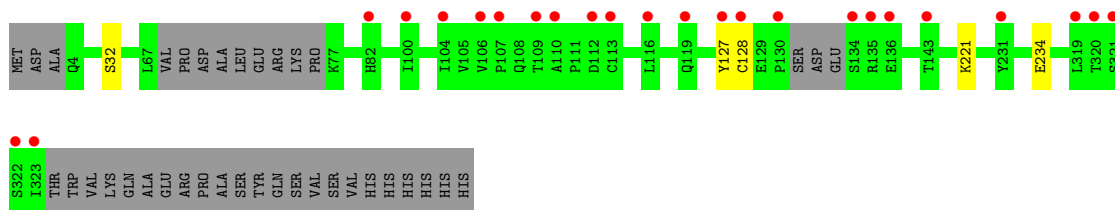
3 Residue-property plots [i](#)

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.

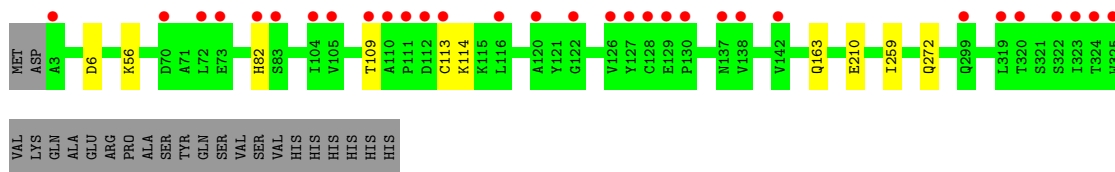
- Molecule 1: Serine racemase



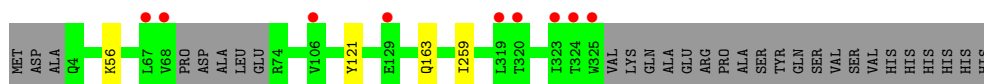
- Molecule 1: Serine racemase



- 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	48.06Å 155.00Å 85.65Å 90.00° 98.26° 90.00°	Depositor
Resolution (Å)	84.76 – 1.80 84.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (84.76-1.80) 97.6 (84.76-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.179 , 0.220 0.179 , 0.220	Depositor DCC
R_{free} test set	5508 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10905	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.47% 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: CA, LLP, EDO, MG, NA, GOL, DMS, PGE

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	0.41	0/2604	0.70	1/3549 (0.0%)
1	BBB	0.32	0/2402	0.64	0/3281
1	CCC	0.33	0/2542	0.66	0/3470
1	DDD	0.36	0/2503	0.65	1/3416 (0.0%)
All	All	0.36	0/10051	0.66	2/13716 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	163	GLN	CB-CG-CD	5.36	125.55	111.60
1	DDD	121	TYR	CB-CA-C	5.14	120.68	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	127[A]	TYR	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	2583	0	2570	0	0
1	BBB	2386	0	2300	0	0
1	CCC	2522	0	2491	0	0
1	DDD	2484	0	2464	0	0
2	AAA	4	0	5	0	0
2	CCC	15	0	18	0	0
2	DDD	18	0	23	0	0
3	AAA	4	0	6	0	0
3	DDD	4	0	6	0	0
4	AAA	1	0	0	0	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	3	0	0	0	0
6	BBB	2	0	0	0	0
6	DDD	1	0	0	0	0
7	AAA	16	0	24	0	0
7	BBB	4	0	6	0	0
7	CCC	16	0	24	0	0
7	DDD	20	0	30	0	0
8	AAA	6	0	8	0	0
8	CCC	18	0	24	0	0
9	AAA	280	0	0	0	0
9	BBB	102	0	0	0	0
9	CCC	190	0	0	0	0
9	DDD	222	0	0	0	0
All	All	10905	0	9999	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	340/346 (98%)	333 (98%)	7 (2%)	0	100	100
1	BBB	319/346 (92%)	309 (97%)	9 (3%)	1 (0%)	41	27
1	CCC	337/346 (97%)	331 (98%)	6 (2%)	0	100	100
1	DDD	327/346 (94%)	319 (98%)	8 (2%)	0	100	100
All	All	1323/1384 (96%)	1292 (98%)	30 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	128	CYS

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	278/290 (96%)	271 (98%)	7 (2%)	47	34
1	BBB	240/290 (83%)	237 (99%)	3 (1%)	69	62
1	CCC	266/290 (92%)	256 (96%)	10 (4%)	33	18
1	DDD	262/290 (90%)	259 (99%)	3 (1%)	73	68
All	All	1046/1160 (90%)	1023 (98%)	23 (2%)	55	39

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	20	ARG
1	AAA	108[A]	GLN
1	AAA	108[B]	GLN
1	AAA	121	TYR
1	AAA	163	GLN
1	AAA	320	THR
1	AAA	325	TRP
1	BBB	32	SER
1	BBB	221	LYS
1	BBB	234	GLU
1	CCC	6	ASP
1	CCC	82[A]	HIS
1	CCC	82[B]	HIS
1	CCC	109	THR
1	CCC	113	CYS
1	CCC	114	LYS
1	CCC	163	GLN
1	CCC	210	GLU
1	CCC	259	ILE
1	CCC	272	GLN
1	DDD	163	GLN
1	DDD	259[A]	ILE
1	DDD	259[B]	ILE

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	AAA	56	1	23,24,25	0.48	0	25,32,34	0.88	1 (4%)
1	LLP	DDD	56	1	23,24,25	0.38	0	25,32,34	0.98	1 (4%)
1	LLP	CCC	56	1	23,24,25	0.52	0	25,32,34	0.92	1 (4%)
1	LLP	BBB	56	1	23,24,25	0.42	0	25,32,34	0.68	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
1	LLP	AAA	56	1	-	2/16/17/19	0/1/1/1
1	LLP	DDD	56	1	-	1/16/17/19	0/1/1/1
1	LLP	CCC	56	1	-	3/16/17/19	0/1/1/1
1	LLP	BBB	56	1	-	1/16/17/19	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	56	LLP	OP4-C5'-C5	3.22	115.49	109.35
1	AAA	56	LLP	OP4-C5'-C5	3.00	115.06	109.35
1	CCC	56	LLP	OP4-C5'-C5	2.22	113.57	109.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BBB	56	LLP	C4-C4'-NZ-CE
1	CCC	56	LLP	C4-C4'-NZ-CE
1	DDD	56	LLP	C4-C4'-NZ-CE
1	AAA	56	LLP	C4-C4'-NZ-CE
1	CCC	56	LLP	CD-CE-NZ-C4'
1	CCC	56	LLP	C-CA-CB-CG
1	AAA	56	LLP	CD-CE-NZ-C4'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 11 are monoatomic - leaving 25 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	$\# Z > 2$
2	PGE	DDD	410	-	9,9,9	0.15	0	8,8,8	0.16	0
7	EDO	DDD	409	-	3,3,3	0.05	0	2,2,2	0.22	0
7	EDO	AAA	407	-	3,3,3	0.23	0	2,2,2	0.34	0
2	PGE	CCC	402	-	4,4,9	0.18	0	3,3,8	0.30	0
8	GOL	CCC	409	-	5,5,5	0.06	0	5,5,5	0.29	0
3	DMS	DDD	404	-	3,3,3	0.40	0	3,3,3	0.03	0
7	EDO	BBB	401	-	3,3,3	0.04	0	2,2,2	0.18	0
7	EDO	DDD	405	-	3,3,3	0.22	0	2,2,2	0.13	0
2	PGE	CCC	410	-	9,9,9	0.18	0	8,8,8	0.08	0
7	EDO	AAA	409	-	3,3,3	0.02	0	2,2,2	0.29	0
8	GOL	AAA	410	-	5,5,5	0.09	0	5,5,5	0.38	0
7	EDO	CCC	406	-	3,3,3	0.03	0	2,2,2	0.09	0
3	DMS	AAA	402	-	3,3,3	0.50	0	3,3,3	0.09	0
7	EDO	CCC	405	-	3,3,3	0.10	0	2,2,2	0.39	0
7	EDO	DDD	406	-	3,3,3	0.07	0	2,2,2	0.16	0
8	GOL	CCC	407	-	5,5,5	0.08	0	5,5,5	0.34	0
7	EDO	AAA	408	-	3,3,3	0.20	0	2,2,2	0.25	0
7	EDO	CCC	404	6	3,3,3	0.10	0	2,2,2	0.31	0
7	EDO	DDD	408	-	3,3,3	0.06	0	2,2,2	0.09	0
7	EDO	DDD	407	-	3,3,3	0.10	0	2,2,2	0.35	0
7	EDO	AAA	406	-	3,3,3	0.19	0	2,2,2	0.11	0
2	PGE	AAA	401	-	3,3,9	0.15	0	2,2,8	0.27	0
8	GOL	CCC	401	-	5,5,5	0.11	0	5,5,5	0.38	0
2	PGE	DDD	403	-	7,7,9	0.24	0	6,6,8	0.17	0
7	EDO	CCC	408	-	3,3,3	0.03	0	2,2,2	0.06	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
2	PGE	DDD	410	-	-	5/7/7/7	-
7	EDO	DDD	409	-	-	1/1/1/1	-
7	EDO	AAA	407	-	-	1/1/1/1	-
2	PGE	CCC	402	-	-	1/2/2/7	-
8	GOL	CCC	409	-	-	2/4/4/4	-
7	EDO	BBB	401	-	-	0/1/1/1	-
7	EDO	DDD	405	-	-	1/1/1/1	-
2	PGE	CCC	410	-	-	5/7/7/7	-
7	EDO	AAA	409	-	-	1/1/1/1	-
8	GOL	AAA	410	-	-	0/4/4/4	-
7	EDO	CCC	406	-	-	0/1/1/1	-
7	EDO	CCC	405	-	-	1/1/1/1	-
7	EDO	DDD	406	-	-	1/1/1/1	-
8	GOL	CCC	407	-	-	2/4/4/4	-
7	EDO	AAA	408	-	-	0/1/1/1	-
7	EDO	CCC	404	6	-	1/1/1/1	-
7	EDO	DDD	408	-	-	0/1/1/1	-
7	EDO	DDD	407	-	-	0/1/1/1	-
7	EDO	AAA	406	-	-	1/1/1/1	-
2	PGE	AAA	401	-	-	1/1/1/7	-
8	GOL	CCC	401	-	-	3/4/4/4	-
2	PGE	DDD	403	-	-	3/5/5/7	-
7	EDO	CCC	408	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	CCC	401	GOL	O1-C1-C2-O2
8	CCC	401	GOL	O1-C1-C2-C3
2	DDD	403	PGE	O2-C3-C4-O3
2	CCC	410	PGE	O1-C1-C2-O2
2	DDD	403	PGE	O1-C1-C2-O2
8	CCC	407	GOL	O1-C1-C2-C3
8	CCC	409	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	DDD	410	PGE	O3-C5-C6-O4
2	AAA	401	PGE	O1-C1-C2-O2
8	CCC	407	GOL	O1-C1-C2-O2
2	DDD	410	PGE	C4-C3-O2-C2
7	AAA	407	EDO	O1-C1-C2-O2
2	CCC	410	PGE	O2-C3-C4-O3
2	CCC	410	PGE	C3-C4-O3-C5
8	CCC	401	GOL	O2-C2-C3-O3
2	CCC	402	PGE	C4-C3-O2-C2
7	AAA	409	EDO	O1-C1-C2-O2
2	CCC	410	PGE	C4-C3-O2-C2
2	CCC	410	PGE	C1-C2-O2-C3
2	DDD	403	PGE	C1-C2-O2-C3
7	CCC	404	EDO	O1-C1-C2-O2
7	DDD	409	EDO	O1-C1-C2-O2
8	CCC	409	GOL	O2-C2-C3-O3
7	AAA	406	EDO	O1-C1-C2-O2
7	DDD	405	EDO	O1-C1-C2-O2
7	DDD	406	EDO	O1-C1-C2-O2
2	DDD	410	PGE	C1-C2-O2-C3
7	CCC	405	EDO	O1-C1-C2-O2
7	CCC	408	EDO	O1-C1-C2-O2
2	DDD	410	PGE	O2-C3-C4-O3
2	DDD	410	PGE	C6-C5-O3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	321/346 (92%)	-0.15	9 (2%) 53 47	12, 20, 51, 105	0
1	BBB	307/346 (88%)	0.18	24 (7%) 13 10	22, 38, 89, 110	0
1	CCC	322/346 (93%)	0.17	31 (9%) 8 6	18, 33, 74, 120	0
1	DDD	316/346 (91%)	-0.08	9 (2%) 53 47	15, 26, 75, 117	0
All	All	1266/1384 (91%)	0.03	73 (5%) 23 18	12, 29, 76, 120	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	320	THR	9.7
1	AAA	319	LEU	7.3
1	CCC	109	THR	7.2
1	BBB	109	THR	6.7
1	CCC	323	ILE	6.2
1	AAA	325	TRP	5.6
1	CCC	322	SER	5.5
1	AAA	323	ILE	5.3
1	BBB	106	VAL	5.2
1	DDD	319	LEU	5.1
1	DDD	324	THR	5.1
1	CCC	325	TRP	5.1
1	CCC	110	ALA	4.9
1	CCC	319	LEU	4.9
1	DDD	325	TRP	4.9
1	AAA	320	THR	4.8
1	AAA	322	SER	4.5
1	CCC	113	CYS	4.2
1	CCC	299[A]	GLN	4.2
1	BBB	127[A]	TYR	4.2
1	BBB	135	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	134	SER	4.0
1	BBB	322	SER	4.0
1	BBB	321	SER	3.9
1	CCC	324	THR	3.9
1	CCC	142[A]	VAL	3.9
1	BBB	104	ILE	3.8
1	BBB	82	HIS	3.7
1	DDD	323	ILE	3.7
1	CCC	72	LEU	3.7
1	BBB	231[A]	TYR	3.3
1	BBB	319	LEU	3.3
1	DDD	68	VAL	3.2
1	BBB	143	THR	3.2
1	CCC	73	GLU	3.2
1	CCC	138	VAL	3.1
1	BBB	128	CYS	3.1
1	AAA	324	THR	3.1
1	BBB	320	THR	3.1
1	CCC	122	GLY	3.0
1	CCC	120	ALA	3.0
1	CCC	127	TYR	2.9
1	BBB	136[A]	GLU	2.9
1	BBB	130	PRO	2.9
1	CCC	320	THR	2.8
1	CCC	111	PRO	2.7
1	CCC	70	ASP	2.7
1	DDD	106	VAL	2.7
1	BBB	116	LEU	2.7
1	AAA	321	SER	2.7
1	BBB	323	ILE	2.6
1	DDD	129	GLU	2.5
1	BBB	113	CYS	2.5
1	CCC	126	VAL	2.4
1	CCC	112	ASP	2.4
1	BBB	100[A]	ILE	2.4
1	CCC	128	CYS	2.3
1	BBB	110	ALA	2.3
1	CCC	104	ILE	2.3
1	AAA	137	ASN	2.3
1	CCC	137	ASN	2.2
1	CCC	129	GLU	2.2
1	AAA	108[A]	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	105[A]	VAL	2.2
1	CCC	82[A]	HIS	2.1
1	BBB	112	ASP	2.1
1	CCC	3[A]	ALA	2.1
1	BBB	107	PRO	2.1
1	DDD	67	LEU	2.0
1	BBB	119	GLN	2.0
1	CCC	130	PRO	2.0
1	CCC	116	LEU	2.0
1	CCC	83[A]	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	BBB	56	24/25	0.97	0.08	25,26,30,32	0
1	LLP	AAA	56	24/25	0.98	0.09	11,14,18,18	0
1	LLP	CCC	56	24/25	0.98	0.08	16,19,21,23	0
1	LLP	DDD	56	24/25	0.98	0.09	15,19,20,21	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
6	NA	AAA	412	1/1	0.53	0.16	60,60,60,60	0
7	EDO	AAA	409	4/4	0.65	0.17	57,57,59,62	0
2	PGE	CCC	410	10/10	0.69	0.28	59,67,74,74	0
2	PGE	DDD	410	10/10	0.72	0.28	59,64,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PGE	AAA	401	4/10	0.76	0.24	49,51,56,58	0
2	PGE	CCC	402	5/10	0.76	0.31	58,58,60,60	0
7	EDO	DDD	406	4/4	0.79	0.28	59,60,63,65	0
8	GOL	CCC	407	6/6	0.80	0.23	54,57,58,58	0
7	EDO	DDD	408	4/4	0.81	0.18	59,60,61,65	0
7	EDO	AAA	407	4/4	0.84	0.19	33,35,35,44	0
7	EDO	CCC	406	4/4	0.84	0.15	57,57,58,58	0
8	GOL	CCC	401	6/6	0.84	0.19	40,43,44,46	0
7	EDO	CCC	408	4/4	0.84	0.16	53,54,56,60	0
7	EDO	BBB	401	4/4	0.85	0.12	62,62,63,63	0
8	GOL	AAA	410	6/6	0.85	0.17	49,53,54,56	0
6	NA	BBB	404	1/1	0.87	0.11	65,65,65,65	0
2	PGE	DDD	403	8/10	0.87	0.17	36,51,54,58	0
7	EDO	AAA	408	4/4	0.87	0.20	37,39,42,44	0
7	EDO	DDD	409	4/4	0.89	0.13	49,52,56,58	0
7	EDO	DDD	405	4/4	0.89	0.22	33,38,43,47	0
7	EDO	AAA	406	4/4	0.89	0.19	43,45,49,54	0
7	EDO	CCC	405	4/4	0.89	0.15	49,51,51,52	0
8	GOL	CCC	409	6/6	0.90	0.22	48,51,51,52	0
7	EDO	CCC	404	4/4	0.92	0.14	39,44,46,53	0
7	EDO	DDD	407	4/4	0.92	0.15	38,41,41,41	0
6	NA	BBB	403	1/1	0.94	0.07	38,38,38,38	0
3	DMS	DDD	404	4/4	0.94	0.13	35,39,39,43	0
4	MG	AAA	403	1/1	0.94	0.10	50,50,50,50	0
3	DMS	AAA	402	4/4	0.94	0.14	26,30,31,34	0
6	NA	AAA	405	1/1	0.98	0.09	24,24,24,24	0
6	NA	DDD	401	1/1	0.98	0.20	39,39,39,39	0
5	CA	BBB	402	1/1	0.98	0.05	35,35,35,35	0
5	CA	CCC	403	1/1	0.98	0.08	27,27,27,27	0
5	CA	AAA	404	1/1	0.99	0.09	15,15,15,15	0
6	NA	AAA	411	1/1	0.99	0.05	19,19,19,19	0
5	CA	DDD	402	1/1	0.99	0.06	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.