



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:44 PM UTC

PDB ID : 6CCZ / pdb_00006ccz
Title : Crystal structure of Medicago truncatula serine hydroxymethyltransferase 3 (MtSHMT3) soaked with selenourea
Authors : Ruszkowski, M.; Sekula, B.; Ruszkowska, A.; Dauter, Z.
Deposited on : 2018-02-07
Resolution : 2.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

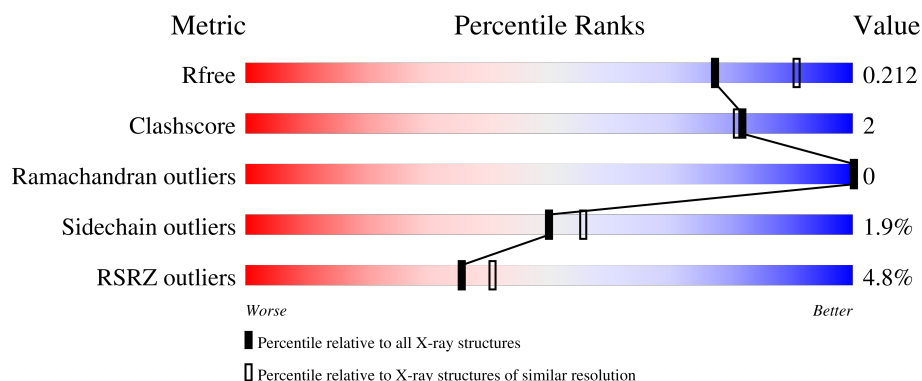
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	A	455	3% 90% 7%
2	B	455	6% 90% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	612	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7226 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 hydroxymethyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	P	S	0	0	0
			3415	2165	592	643	1	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	SER	-	expression tag	UNP G7ILW0
A	80	ASN	-	expression tag	UNP G7ILW0
A	81	ALA	-	expression tag	UNP G7ILW0

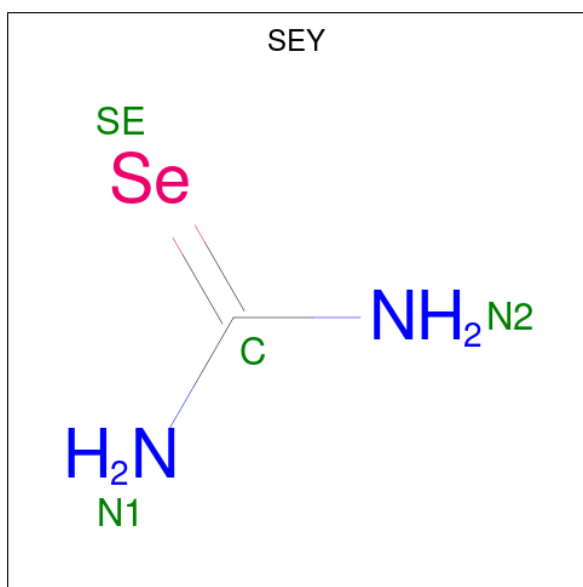
- Molecule 2 is a protein called Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	0	0
			3392	2153	590	635	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	SER	-	expression tag	UNP G7ILW0
B	80	ASN	-	expression tag	UNP G7ILW0
B	81	ALA	-	expression tag	UNP G7ILW0

- Molecule 3 is selenourea (CCD ID: SEY) (formula: CH₄N₂Se).



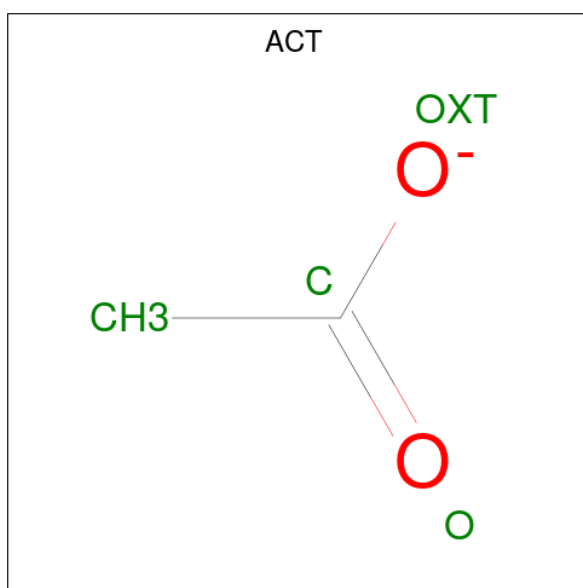
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	Se	0	0
			4	1	2	1		
3	A	1	Total	C	N	Se	0	0
			4	1	2	1		
3	A	1	Total	C	N	Se	0	0
			4	1	2	1		
3	A	1	Total	C	N	Se	0	0
			4	1	2	1		
3	A	1	Total	C	N	Se	0	0
			4	1	2	1		
3	A	1	Total	C	N	Se	0	0
			4	1	2	1		
3	A	1	Total	C	N	Se	0	0
			4	1	2	1		
3	A	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	Se	0	0
			4	1	2	1		
3	B	1	Total	C	N	Se	0	0
			4	1	2	1		
3	B	1	Total	C	N	Se	0	0
			4	1	2	1		
3	B	1	Total	C	N	Se	0	0
			4	1	2	1		
3	B	1	Total	C	N	Se	0	0
			4	1	2	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

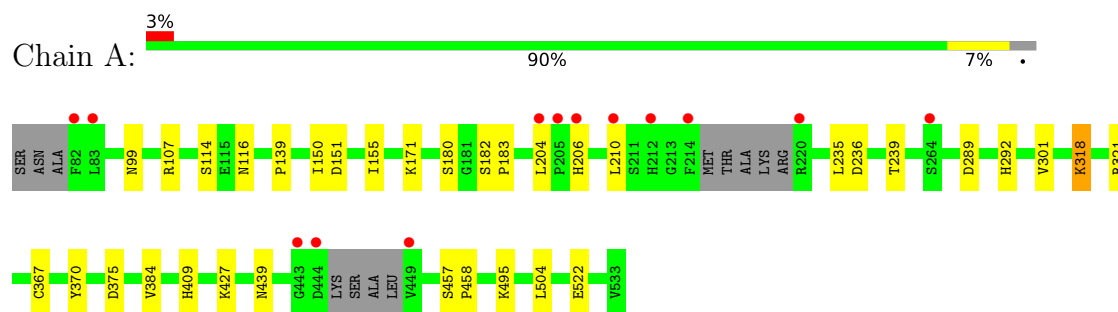
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total	O	0	0
			176	176		
6	B	149	Total	O	0	0
			149	149		

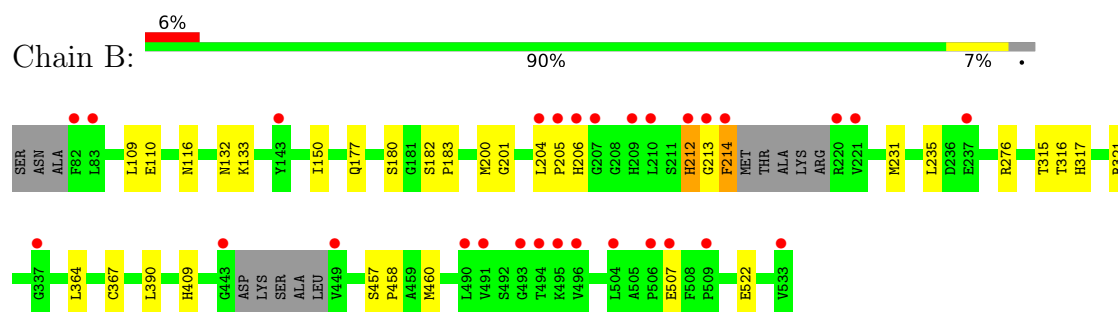
3 Residue-property plots [i](#)

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 hydroxymethyltransferase



- Molecule 2: Serine hydroxymethyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.67Å 199.69Å 152.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.53 – 2.14 83.53 – 2.14	Depositor EDS
% Data completeness (in resolution range)	95.7 (83.53-2.14) 97.0 (83.53-2.14)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.165 , 0.206 0.175 , 0.212	Depositor DCC
R_{free} test set	1007 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.7	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	0.96	EDS
Total number of atoms	7226	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 3.51% 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: LLP, FMT, ACT, SEY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	1/3460 (0.0%)	0.97	0/4679
2	B	0.93	1/3462 (0.0%)	1.00	6/4682 (0.1%)
All	All	0.96	2/6922 (0.0%)	0.99	6/9361 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	522	GLU	C-O	-5.26	1.17	1.24
1	A	204	LEU	CA-C	5.14	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	212	HIS	CA-C-N	5.92	126.56	119.98
2	B	212	HIS	C-N-CA	5.92	126.56	119.98
2	B	212	HIS	CB-CA-C	-5.85	107.09	114.40
2	B	177	GLN	CA-C-N	-5.31	114.29	119.76
2	B	177	GLN	C-N-CA	-5.31	114.29	119.76
2	B	132	ASN	N-CA-C	5.18	119.45	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3415	0	3389	18	0
2	B	3392	0	3380	16	0
3	A	44	0	0	0	0
3	B	32	0	0	0	0
4	A	4	0	3	3	0
4	B	8	0	6	0	0
5	A	3	0	1	0	0
5	B	3	0	1	0	0
6	A	176	0	0	0	0
6	B	149	0	0	1	0
All	All	7226	0	6780	34	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (34) 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:A:409:HIS:H	1:A:409:HIS:CD2	2.23	0.56
2:B:214:PHE:C	2:B:214:PHE:CD1	2.85	0.54
1:A:206:HIS:HB3	1:A:235:LEU:HG	1.89	0.53
1:A:301:VAL:HG11	1:A:384:VAL:HG21	1.91	0.53
2:B:206:HIS:HB3	2:B:235:LEU:HG	1.89	0.53
1:A:151:ASP:O	1:A:155:ILE:HG12	2.10	0.52
2:B:201:GLY:N	2:B:213:GLY:HA3	2.23	0.52
1:A:292:HIS:ND1	1:A:318:LLP:O3	2.44	0.51
2:B:276:ARG:NH2	6:B:701:HOH:O	2.37	0.50
2:B:109:LEU:HD23	2:B:460:MET:HE2	1.95	0.49
1:A:427:LYS:HE3	1:A:504:LEU:HD21	1.94	0.48
1:A:116:ASN:ND2	1:A:321:ARG:HG2	2.29	0.47
2:B:409:HIS:H	2:B:409:HIS:CD2	2.32	0.47
1:A:318:LLP:C4'	4:A:612:ACT:H2	2.45	0.47
2:B:133:LYS:HG2	2:B:150:ILE:HG13	1.96	0.47
1:A:289:ASP:OD2	1:A:318:LLP:N1	2.48	0.46
1:A:318:LLP:H4'1	4:A:612:ACT:H2	1.97	0.46
1:A:236:ASP:HB3	1:A:239:THR:OG1	2.16	0.46
2:B:214:PHE:CD1	2:B:214:PHE:O	2.69	0.45
1:A:107:ARG:O	1:A:522:GLU:HG2	2.17	0.44
2:B:200:MET:HE3	2:B:231:MET:HE2	1.99	0.44
1:A:206:HIS:O	1:A:235:LEU:HD11	2.19	0.43
2:B:212:HIS:HB3	2:B:213:GLY:H	1.56	0.42
1:A:457:SER:N	1:A:458:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:THR:HG21	2:B:364:LEU:HD13	2.02	0.41
1:A:182:SER:HB2	1:A:183:PRO:HD3	2.02	0.41
1:A:114:SER:OG	4:A:612:ACT:O	2.38	0.41
2:B:204:LEU:HB3	2:B:205:PRO:HD3	2.03	0.41
1:A:370:TYR:OH	1:A:375:ASP:OD2	2.33	0.41
2:B:182:SER:HB2	2:B:183:PRO:HD3	2.03	0.41
2:B:315:THR:HB	2:B:317:HIS:CE1	2.56	0.41
1:A:139:PRO:HB2	1:A:155:ILE:HD11	2.01	0.40
2:B:457:SER:N	2:B:458:PRO:CD	2.85	0.40
2:B:116:ASN:ND2	2:B:321:ARG:HG2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/455 (96%)	421 (97%)	15 (3%)	0	100	100
2	B	436/455 (96%)	417 (96%)	19 (4%)	0	100	100
All	All	872/910 (96%)	838 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/371 (98%)	354 (98%)	8 (2%)	45	49
2	B	362/372 (97%)	356 (98%)	6 (2%)	53	58
All	All	724/743 (97%)	710 (98%)	14 (2%)	50	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	150	ILE
1	A	171	LYS
1	A	180	SER
1	A	210	LEU
1	A	367	CYS
1	A	439	ASN
1	A	495	LYS
2	B	110	GLU
2	B	180	SER
2	B	214	PHE
2	B	367	CYS
2	B	390	LEU
2	B	507	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	A	409	HIS
1	A	497	GLN
1	A	501	ASN
2	B	166	HIS
2	B	382	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	A	318	1	23,24,25	1.38	3 (13%)	25,32,34	1.72	5 (20%)

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	A	318	1	-	10/16/17/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	LLP	C4-C4'	3.41	1.53	1.46
1	A	318	LLP	C2'-C2	2.78	1.54	1.50
1	A	318	LLP	O3-C3	2.58	1.42	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	LLP	CE-NZ-C4'	4.43	132.89	118.72
1	A	318	LLP	OP4-C5'-C5	3.58	116.07	109.36
1	A	318	LLP	C5'-C5-C6	-3.19	114.16	119.36
1	A	318	LLP	C4-C4'-NZ	-2.64	111.84	124.04
1	A	318	LLP	C5-C6-N1	-2.21	120.24	123.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	318	LLP	C4-C5-C5'-OP4
1	A	318	LLP	C6-C5-C5'-OP4
1	A	318	LLP	C5'-OP4-P-OP3

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Mol	Chain	Res	Type	Atoms
1	A	318	LLP	O-C-CA-CB
1	A	318	LLP	C5'-OP4-P-OP2
1	A	318	LLP	CD-CE-NZ-C4'
1	A	318	LLP	C5'-OP4-P-OP1
1	A	318	LLP	C3-C4-C4'-NZ
1	A	318	LLP	C5-C4-C4'-NZ
1	A	318	LLP	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	318	LLP	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SEY	A	605	-	3,3,3	0.53	0	3,3,3	0.51	0
3	SEY	A	603	-	3,3,3	0.35	0	3,3,3	0.17	0
3	SEY	B	605	-	3,3,3	0.39	0	3,3,3	0.14	0
3	SEY	A	604	-	3,3,3	0.44	0	3,3,3	0.12	0
3	SEY	A	609	-	3,3,3	0.33	0	3,3,3	0.16	0
3	SEY	A	602	-	3,3,3	0.57	0	3,3,3	0.28	0
3	SEY	B	604	-	3,3,3	0.82	0	3,3,3	0.05	0
4	ACT	B	610	-	3,3,3	0.91	0	3,3,3	0.65	0
3	SEY	B	602	-	3,3,3	0.25	0	3,3,3	1.39	0
4	ACT	B	609	-	3,3,3	0.99	0	3,3,3	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	A	612	-	3,3,3	0.81	0	3,3,3	1.04	0
3	SEY	A	601	-	3,3,3	0.69	0	3,3,3	0.16	0
3	SEY	A	607	-	3,3,3	0.65	0	3,3,3	0.65	0
5	FMT	B	611	-	2,2,2	0.46	0	1,1,1	0.42	0
3	SEY	A	611	-	3,3,3	0.69	0	3,3,3	0.09	0
3	SEY	B	601	-	3,3,3	0.23	0	3,3,3	0.46	0
3	SEY	B	607	-	3,3,3	0.76	0	3,3,3	0.25	0
5	FMT	A	613	-	2,2,2	0.49	0	1,1,1	0.66	0
3	SEY	A	606	-	3,3,3	0.65	0	3,3,3	0.22	0
3	SEY	A	608	-	3,3,3	0.15	0	3,3,3	0.32	0
3	SEY	B	606	-	3,3,3	0.73	0	3,3,3	0.15	0
3	SEY	B	608	-	3,3,3	0.61	0	3,3,3	0.18	0
3	SEY	B	603	-	3,3,3	0.73	0	3,3,3	0.08	0
3	SEY	A	610	-	3,3,3	0.66	0	3,3,3	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	612	ACT	3	0

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	A	442/455 (97%)	-0.16	13 (2%) 53 57	20, 30, 52, 91	0
2	B	442/455 (97%)	0.13	29 (6%) 24 28	22, 34, 67, 99	0
All	All	884/910 (97%)	-0.01	42 (4%) 35 41	20, 32, 62, 99	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	82	PHE	7.5
2	B	214	PHE	6.9
2	B	213	GLY	6.9
1	A	82	PHE	6.7
2	B	83	LEU	6.7
2	B	204	LEU	5.0
2	B	212	HIS	4.5
1	A	83	LEU	4.2
2	B	210	LEU	4.2
1	A	205	PRO	3.9
2	B	206	HIS	3.9
2	B	443	GLY	3.9
1	A	214	PHE	3.7
2	B	205	PRO	3.7
2	B	506	PRO	3.7
1	A	444	ASP	3.5
2	B	221	VAL	3.1
2	B	494	THR	3.1
2	B	504	LEU	3.1
1	A	449	VAL	2.9
1	A	443	GLY	2.9
2	B	449	VAL	2.9
2	B	220	ARG	2.9
2	B	209	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	212	HIS	2.8
2	B	533	VAL	2.8
2	B	237	GLU	2.7
2	B	507	GLU	2.7
1	A	206	HIS	2.7
2	B	491	VAL	2.5
1	A	210	LEU	2.5
2	B	143	TYR	2.4
1	A	204	LEU	2.3
2	B	207	GLY	2.3
1	A	264	SER	2.3
2	B	496	VAL	2.3
2	B	490	LEU	2.3
2	B	509	PRO	2.2
2	B	493	GLY	2.2
1	A	220	ARG	2.2
2	B	337	GLY	2.1
2	B	495	LYS	2.1

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	A	318	24/25	0.87	0.15	28,48,52,53	0

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	SEY	A	611	4/4	0.82	0.23	76,77,81,84	0
3	SEY	B	608	4/4	0.82	0.20	80,85,88,89	0
3	SEY	B	607	4/4	0.83	0.20	79,83,83,83	0
4	ACT	A	612	4/4	0.83	0.17	47,54,55,58	0
4	ACT	B	609	4/4	0.83	0.16	48,53,55,56	0
4	ACT	B	610	4/4	0.83	0.17	47,50,50,51	0
3	SEY	A	608	4/4	0.84	0.20	62,69,70,80	0
3	SEY	A	602	4/4	0.88	0.25	56,61,62,65	0
3	SEY	A	610	4/4	0.88	0.17	77,80,83,94	0
3	SEY	B	602	4/4	0.90	0.19	73,74,75,79	4
3	SEY	A	607	4/4	0.91	0.26	58,59,64,67	0
3	SEY	B	606	4/4	0.92	0.15	67,76,77,77	0
3	SEY	A	609	4/4	0.93	0.21	59,60,61,66	0
3	SEY	B	604	4/4	0.93	0.16	66,71,72,74	0
3	SEY	B	605	4/4	0.93	0.13	75,76,76,78	0
3	SEY	B	601	4/4	0.94	0.19	49,50,51,55	0
3	SEY	B	603	4/4	0.95	0.18	60,63,65,66	0
5	FMT	A	613	3/3	0.95	0.09	35,35,36,37	0
5	FMT	B	611	3/3	0.95	0.10	40,40,45,47	0
3	SEY	A	601	4/4	0.96	0.15	50,51,52,56	4
3	SEY	A	605	4/4	0.97	0.14	44,45,46,49	0
3	SEY	A	606	4/4	0.97	0.16	58,59,60,62	0
3	SEY	A	603	4/4	0.98	0.11	43,45,45,47	0
3	SEY	A	604	4/4	0.98	0.12	45,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.