



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:38 AM UTC

PDB ID : 6O64 / pdb_00006o64
Title : Crystal Structure of Arabidopsis thaliana Spermidine Synthase isoform 2 (At-SPDS2)
Authors : Sekula, B.; Dauter, Z.
Deposited on : 2019-03-05
Resolution : 2.00 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
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

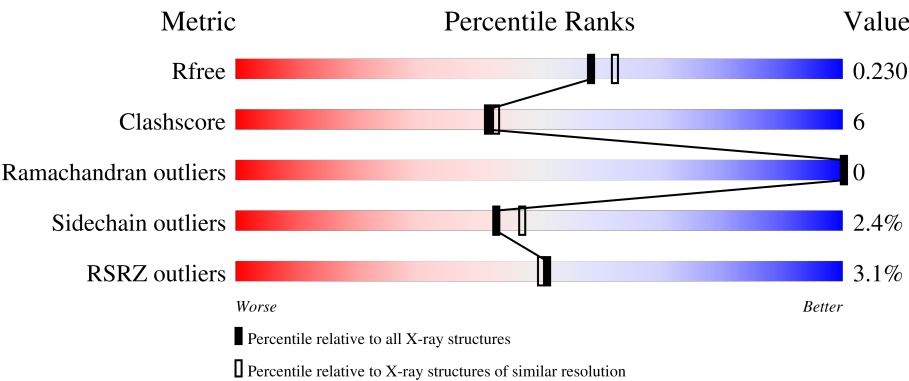
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	305	2% 79%13%• 7%
1	B	305	3% 80%14%5%
1	C	305	2% 77%13%• 9%
1	D	305	8% 70%18%• 10%
1	E	305	2% 71%19%• 8%

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Mol	Chain	Length	Quality of chain
1	F	305	
1	G	305	
1	H	305	

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	EDO	E	402	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18590 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 Spermidine synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	1	0
			2202	1415	354	418	15			
1	B	290	Total	C	N	O	S	0	0	0
			2238	1436	362	425	15			
1	C	277	Total	C	N	O	S	0	0	0
			2145	1378	346	408	13			
1	D	275	Total	C	N	O	S	0	0	0
			2131	1371	344	403	13			
1	E	281	Total	C	N	O	S	0	3	0
			2183	1407	350	411	15			
1	F	287	Total	C	N	O	S	0	2	0
			2223	1430	358	419	16			
1	G	288	Total	C	N	O	S	0	0	0
			2220	1426	357	422	15			
1	H	281	Total	C	N	O	S	0	1	0
			2178	1401	352	411	14			

There are 24 discrepancies between the modelled and reference sequences:

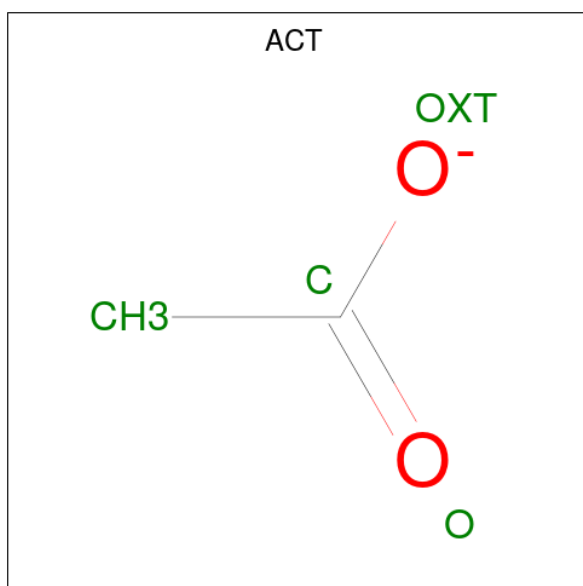
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	SER	-	expression tag	UNP O48661
A	37	ASN	-	expression tag	UNP O48661
A	38	ALA	-	expression tag	UNP O48661
B	36	SER	-	expression tag	UNP O48661
B	37	ASN	-	expression tag	UNP O48661
B	38	ALA	-	expression tag	UNP O48661
C	36	SER	-	expression tag	UNP O48661
C	37	ASN	-	expression tag	UNP O48661
C	38	ALA	-	expression tag	UNP O48661
D	36	SER	-	expression tag	UNP O48661
D	37	ASN	-	expression tag	UNP O48661
D	38	ALA	-	expression tag	UNP O48661
E	36	SER	-	expression tag	UNP O48661

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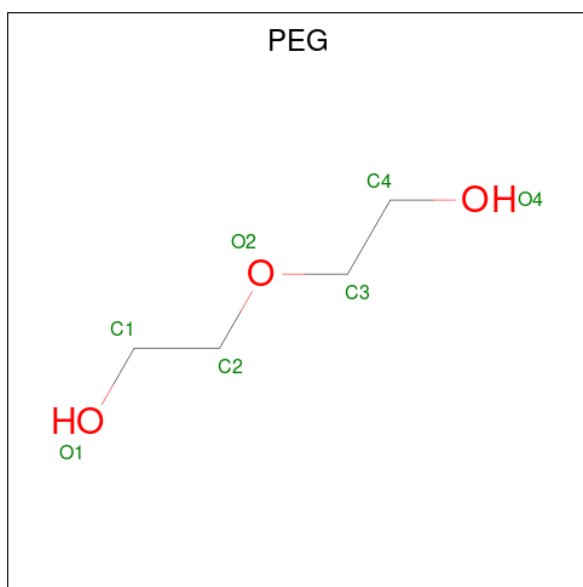
Chain	Residue	Modelled	Actual	Comment	Reference
E	37	ASN	-	expression tag	UNP O48661
E	38	ALA	-	expression tag	UNP O48661
F	36	SER	-	expression tag	UNP O48661
F	37	ASN	-	expression tag	UNP O48661
F	38	ALA	-	expression tag	UNP O48661
G	36	SER	-	expression tag	UNP O48661
G	37	ASN	-	expression tag	UNP O48661
G	38	ALA	-	expression tag	UNP O48661
H	36	SER	-	expression tag	UNP O48661
H	37	ASN	-	expression tag	UNP O48661
H	38	ALA	-	expression tag	UNP O48661

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



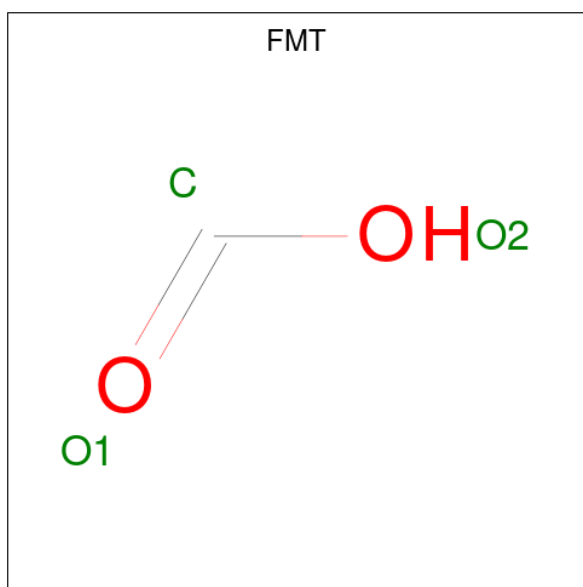
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



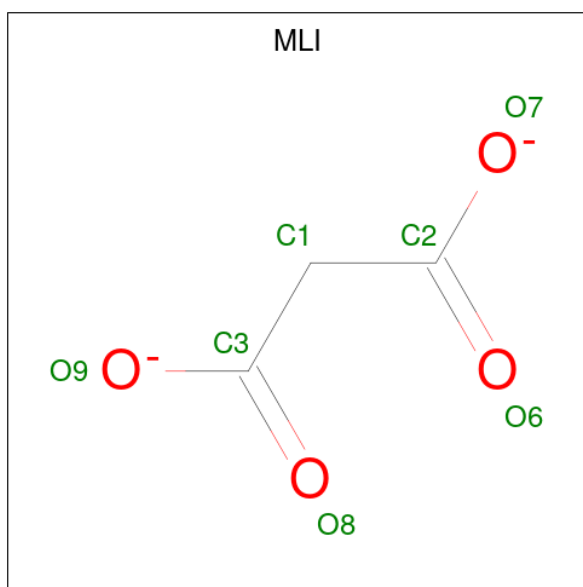
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	1
			6	2	4		

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



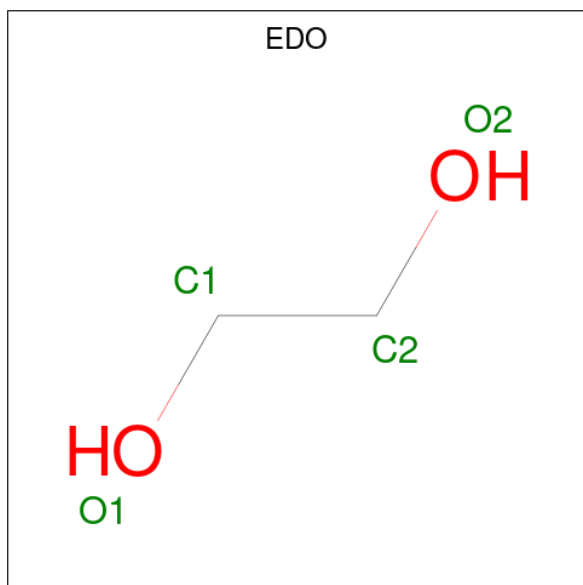
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			7	3	4		
5	E	1	Total	C	O	0	0
			7	3	4		
5	H	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	79	Total	O	0	0
			79	79		
7	B	99	Total	O	0	0
			99	99		
7	C	84	Total	O	0	0
			84	84		
7	D	67	Total	O	0	0
			67	67		
7	E	186	Total	O	0	0
			186	186		

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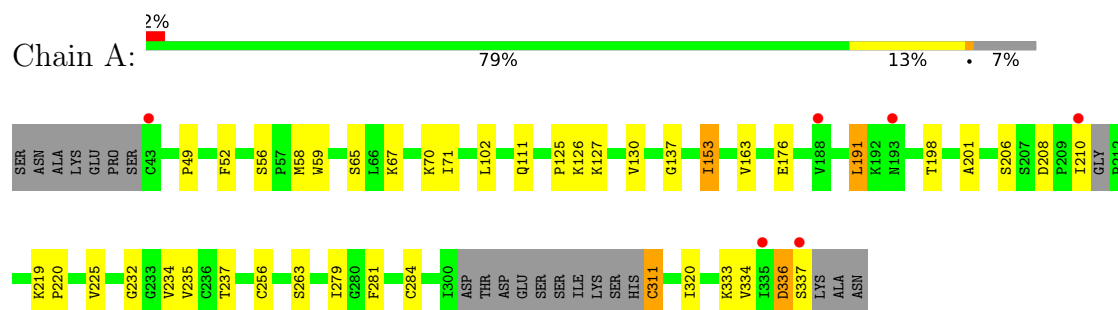
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	162	Total 162	O 162	0	0
7	G	143	Total 143	O 143	0	0
7	H	116	Total 116	O 116	0	0

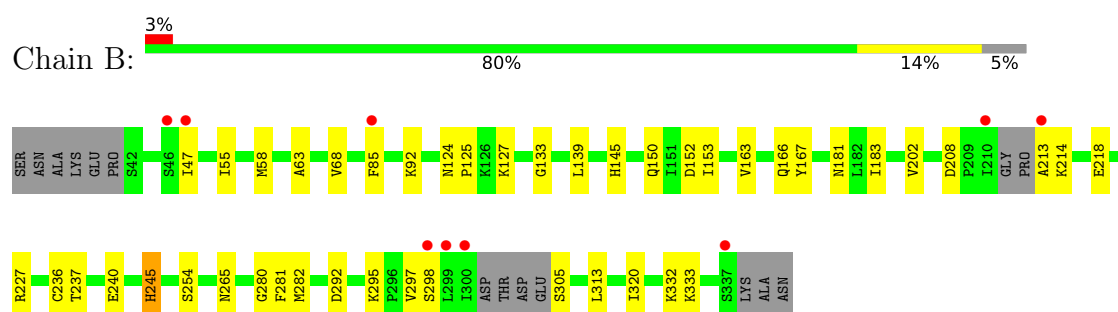
3 Residue-property plots [i](#)

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.

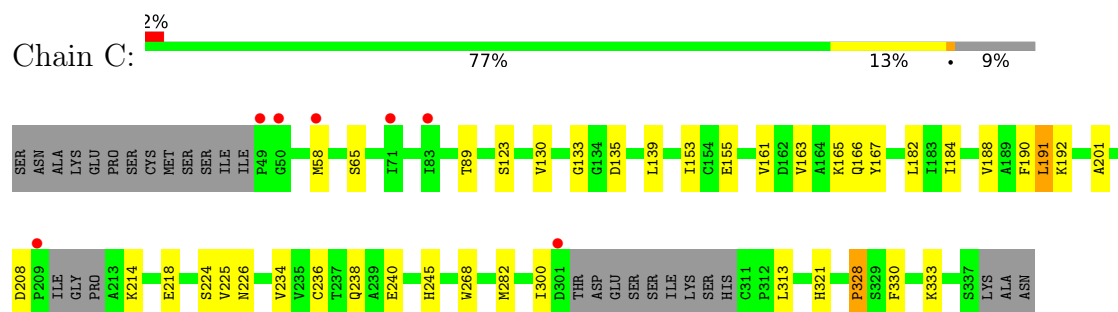
• Molecule 1: Spermidine synthase 2



• Molecule 1: Spermidine synthase 2

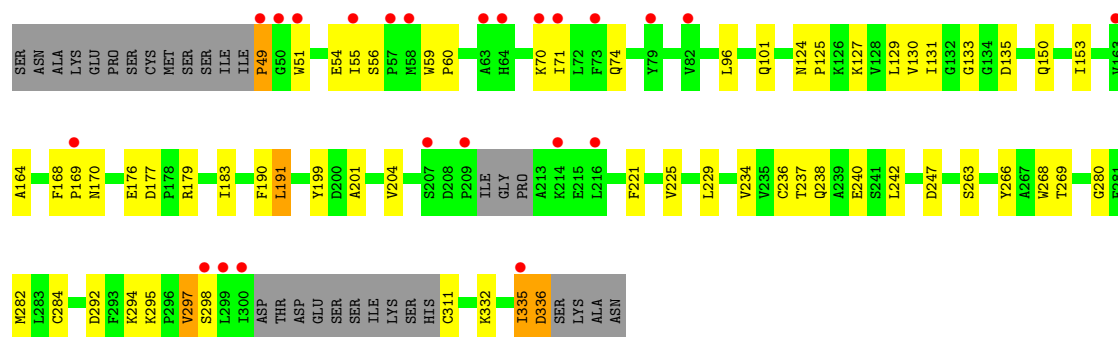


• Molecule 1: Spermidine synthase 2

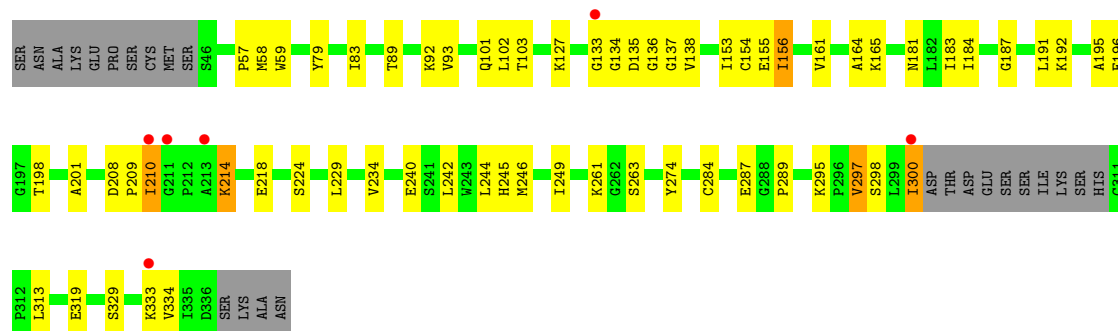


• Molecule 1: Spermidine synthase 2

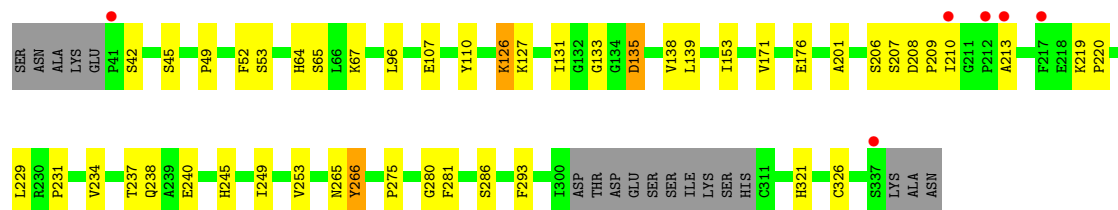
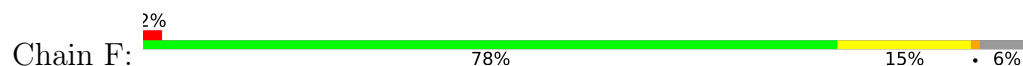




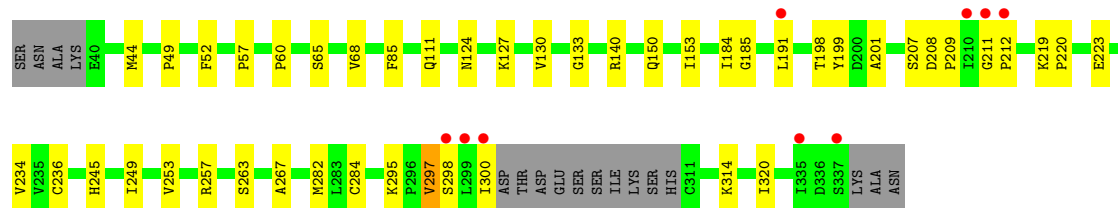
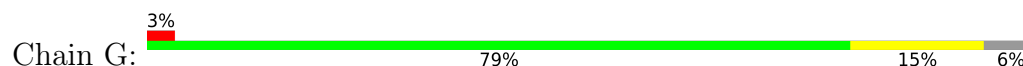
• Molecule 1: Spermidine synthase 2



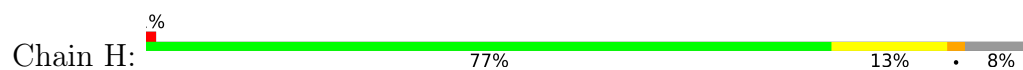
• Molecule 1: Spermidine synthase 2

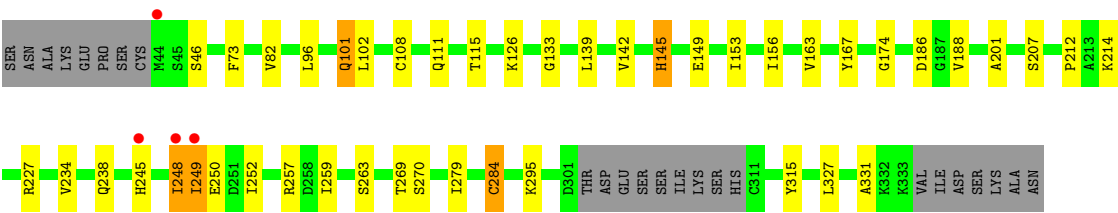


• Molecule 1: Spermidine synthase 2



• Molecule 1: Spermidine synthase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.65Å 162.70Å 97.49Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	42.54 – 2.00 42.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	80.2 (42.54-2.00) 80.2 (42.54-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.231 0.185 , 0.230	Depositor DCC
R_{free} test set	1504 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.1	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	0.95	EDS
Total number of atoms	18590	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: FMT, ACT, MLI, PEG, EDO

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	1.13	0/2252	1.44	6/3056 (0.2%)
1	B	1.22	6/2288 (0.3%)	1.44	3/3103 (0.1%)
1	C	1.15	1/2194 (0.0%)	1.43	5/2977 (0.2%)
1	D	1.16	1/2180 (0.0%)	1.46	4/2958 (0.1%)
1	E	1.30	8/2243 (0.4%)	1.43	8/3046 (0.3%)
1	F	1.34	7/2282 (0.3%)	1.45	7/3098 (0.2%)
1	G	1.25	7/2272 (0.3%)	1.46	9/3086 (0.3%)
1	H	1.32	8/2233 (0.4%)	1.46	2/3032 (0.1%)
All	All	1.24	38/17944 (0.2%)	1.45	44/24356 (0.2%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	171	VAL	C-O	7.60	1.31	1.24
1	E	245	HIS	CE1-NE2	7.48	1.40	1.32
1	H	102	LEU	C-O	7.20	1.32	1.23
1	G	207	SER	C-O	6.94	1.31	1.23
1	G	185	GLY	C-O	6.72	1.30	1.23
1	D	229	LEU	C-O	6.68	1.32	1.23
1	B	245	HIS	CE1-NE2	6.68	1.39	1.32
1	F	326	CYS	C-O	6.58	1.31	1.24
1	H	284	CYS	C-O	6.47	1.31	1.23
1	H	46	SER	C-O	6.37	1.31	1.23
1	F	110	TYR	C-O	-6.32	1.16	1.24
1	G	267	ALA	C-O	6.25	1.31	1.23
1	H	108	CYS	C-O	6.21	1.31	1.24
1	B	320	ILE	C-O	6.17	1.32	1.24
1	B	145	HIS	CE1-NE2	6.16	1.38	1.32
1	H	115	THR	C-O	6.13	1.30	1.24
1	F	53	SER	C-O	-6.09	1.17	1.24
1	F	321	HIS	CE1-NE2	6.04	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	289	PRO	C-O	5.98	1.30	1.23
1	F	266	TYR	C-O	5.89	1.30	1.24
1	B	202	VAL	C-O	-5.83	1.17	1.24
1	B	313	LEU	C-O	5.78	1.30	1.23
1	C	226	ASN	C-O	5.52	1.30	1.24
1	H	315	TYR	CA-C	5.51	1.57	1.52
1	E	83	ILE	C-O	5.43	1.29	1.24
1	E	57	PRO	C-O	-5.41	1.16	1.24
1	G	124	ASN	N-CA	5.39	1.50	1.46
1	H	145	HIS	CE1-NE2	5.33	1.37	1.32
1	E	224[A]	SER	C-O	5.23	1.30	1.24
1	E	224[B]	SER	C-O	5.23	1.30	1.24
1	G	191	LEU	C-O	5.19	1.30	1.24
1	G	49	PRO	C-O	-5.18	1.17	1.23
1	G	245	HIS	CE1-NE2	5.14	1.37	1.32
1	H	270	SER	CA-CB	-5.08	1.45	1.53
1	E	242	LEU	C-O	-5.07	1.17	1.24
1	F	96	LEU	C-O	5.06	1.29	1.24
1	B	152	ASP	C-O	5.05	1.30	1.24
1	E	229	LEU	C-O	5.01	1.29	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	ASP	CA-CB-CG	6.69	119.29	112.60
1	G	184	ILE	CA-C-O	-6.06	117.36	122.63
1	A	336	ASP	N-CA-C	6.04	117.69	109.11
1	G	314	LYS	CB-CA-C	5.94	120.11	109.29
1	G	297	VAL	CA-C-N	5.88	132.49	122.37
1	G	297	VAL	C-N-CA	5.88	132.49	122.37
1	H	249	ILE	CA-C-O	-5.79	114.62	121.05
1	G	85	PHE	CA-CB-CG	5.74	119.54	113.80
1	D	297	VAL	O-C-N	5.72	127.73	121.83
1	H	111	GLN	CA-C-O	-5.67	114.41	120.42
1	E	210	ILE	CB-CA-C	-5.66	103.09	112.26
1	A	125	PRO	CA-C-O	-5.65	115.19	121.23
1	E	210	ILE	N-CA-C	5.65	118.15	111.09
1	G	111	GLN	CA-C-O	-5.62	114.46	120.42
1	B	280	GLY	O-C-N	5.62	128.18	123.29
1	F	138	VAL	N-CA-C	-5.61	105.06	110.72
1	A	256	CYS	CA-C-N	5.56	128.29	120.28
1	A	256	CYS	C-N-CA	5.56	128.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	199	TYR	CA-C-N	5.56	128.18	120.29
1	G	199	TYR	C-N-CA	5.56	128.18	120.29
1	B	213	ALA	CA-C-N	5.48	128.17	120.28
1	B	213	ALA	C-N-CA	5.48	128.17	120.28
1	F	229	LEU	CA-C-N	5.45	128.94	120.60
1	F	229	LEU	C-N-CA	5.45	128.94	120.60
1	F	213	ALA	CA-C-N	5.45	128.33	120.38
1	F	213	ALA	C-N-CA	5.45	128.33	120.38
1	F	275	PRO	CA-C-O	-5.41	115.44	121.23
1	G	223	GLU	CB-CG-CD	5.37	121.72	112.60
1	E	89	THR	CA-CB-OG1	-5.35	101.57	109.60
1	E	196	GLU	CB-CA-C	-5.30	101.23	109.61
1	E	249	ILE	N-CA-C	-5.28	105.39	110.72
1	C	328	PRO	CA-C-N	5.26	127.59	120.38
1	C	328	PRO	C-N-CA	5.26	127.59	120.38
1	E	214	LYS	CA-C-N	5.23	129.58	120.68
1	E	214	LYS	C-N-CA	5.23	129.58	120.68
1	C	321	HIS	CA-C-O	-5.16	114.98	121.02
1	D	247	ASP	CA-C-N	5.11	127.10	120.56
1	D	247	ASP	C-N-CA	5.11	127.10	120.56
1	A	232	GLY	CA-C-N	5.09	125.99	120.44
1	A	232	GLY	C-N-CA	5.09	125.99	120.44
1	E	101	GLN	N-CA-C	-5.06	107.24	113.41
1	F	135	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	190	PHE	CA-CB-CG	-5.04	108.76	113.80
1	D	335	ILE	O-C-N	5.04	127.02	121.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2202	0	2180	23	0
1	B	2238	0	2220	23	0
1	C	2145	0	2117	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2131	0	2108	36	0
1	E	2183	0	2175	51	0
1	F	2223	0	2209	24	0
1	G	2220	0	2198	23	0
1	H	2178	0	2157	34	0
2	A	4	0	3	0	0
2	F	4	0	3	0	0
2	H	12	0	9	0	0
3	A	7	0	10	1	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	D	21	0	30	0	0
3	E	7	0	10	1	0
3	F	14	0	20	2	0
3	G	7	0	10	1	0
4	B	3	0	1	0	0
4	E	9	0	3	0	0
5	D	7	0	2	0	0
5	E	14	0	4	0	0
5	H	7	0	2	0	0
6	E	4	0	6	17	0
7	A	79	0	0	2	0
7	B	99	0	0	2	0
7	C	84	0	0	1	0
7	D	67	0	0	1	0
7	E	186	0	0	3	0
7	F	162	0	0	7	0
7	G	143	0	0	0	0
7	H	116	0	0	5	0
All	All	18590	0	17497	226	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 6.

All (226) 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:E:58[A]:MET:SD	1:E:210:ILE:HG12	2.10	0.91
1:E:138:VAL:H	6:E:402:EDO:C2	1.86	0.87
1:E:138:VAL:H	6:E:402:EDO:H22	1.40	0.87
1:G:127:LYS:HE3	1:G:150:GLN:NE2	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:LYS:HG3	3:F:403:PEG:H12	1.63	0.80
1:A:58:MET:HE2	1:A:208:ASP:HB3	1.63	0.80
1:E:134:GLY:HA3	6:E:402:EDO:H12	1.65	0.77
1:E:137:GLY:N	6:E:402:EDO:H22	2.00	0.77
1:E:135:ASP:N	6:E:402:EDO:H11	2.01	0.76
1:H:126:LYS:HD3	1:H:149:GLU:HG3	1.67	0.76
1:H:133:GLY:HA2	1:H:153:ILE:HD11	1.66	0.76
1:B:127:LYS:HE3	1:B:150:GLN:NE2	2.01	0.75
1:F:133:GLY:HA2	1:F:153:ILE:HD11	1.70	0.74
1:D:71:ILE:HG21	1:D:74:GLN:HE21	1.53	0.73
1:E:136:GLY:H	6:E:402:EDO:H11	1.52	0.72
1:C:58:MET:HE3	1:C:208:ASP:HB3	1.69	0.72
7:B:552:HOH:O	1:E:92:LYS:HE2	1.89	0.72
1:G:44:MET:HE1	1:G:68:VAL:HG21	1.72	0.72
1:H:249:ILE:HD12	1:H:331:ALA:HB1	1.72	0.71
1:A:333:LYS:HG3	1:A:334:VAL:H	1.57	0.69
1:E:134:GLY:HA3	6:E:402:EDO:C1	2.23	0.69
1:H:245:HIS:HB2	1:H:248:ILE:HG13	1.76	0.68
1:H:245:HIS:HB2	1:H:248:ILE:CG1	2.24	0.67
1:D:133:GLY:HA2	1:D:153:ILE:HD11	1.78	0.66
1:C:133:GLY:HA2	1:C:153:ILE:HD11	1.77	0.65
1:D:332:LYS:O	1:D:336:ASP:HB2	1.96	0.65
1:H:139:LEU:HD11	1:H:153:ILE:HD13	1.79	0.64
1:B:214:LYS:HE2	1:B:218:GLU:OE2	1.98	0.64
1:B:133:GLY:HA2	1:B:153:ILE:HD11	1.79	0.63
1:H:126:LYS:HD3	1:H:149:GLU:CG	2.28	0.63
1:F:207:SER:HB2	7:F:617:HOH:O	1.98	0.62
1:B:240:GLU:HB3	1:B:245:HIS:ND1	2.14	0.62
1:D:71:ILE:HG21	1:D:74:GLN:NE2	2.15	0.62
1:F:139:LEU:HD11	1:F:153:ILE:HD13	1.82	0.62
1:G:127:LYS:HE3	1:G:150:GLN:CD	2.24	0.61
1:A:311:CYS:O	1:A:311:CYS:SG	2.58	0.61
1:G:133:GLY:HA2	1:G:153:ILE:HD11	1.81	0.61
1:E:138:VAL:H	6:E:402:EDO:H21	1.64	0.61
1:H:212:PRO:HG3	1:H:248:ILE:HD12	1.82	0.61
1:B:297:VAL:HG23	1:B:298:SER:HB3	1.83	0.61
1:E:127:LYS:HE2	1:E:198:THR:HG22	1.82	0.61
1:C:300:ILE:HG23	1:C:313:LEU:HD11	1.82	0.60
1:D:170:ASN:ND2	1:H:250:GLU:OE2	2.34	0.60
1:E:138:VAL:N	6:E:402:EDO:H22	2.13	0.60
1:H:139:LEU:HD21	1:H:153:ILE:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:MET:HE2	1:E:334:VAL:HG11	1.84	0.59
1:B:68:VAL:HG22	1:B:85:PHE:CD1	2.37	0.59
1:A:219:LYS:HB2	1:A:220:PRO:HD3	1.85	0.58
1:E:135:ASP:H	6:E:402:EDO:C1	2.16	0.58
1:H:238:GLN:HB2	7:H:554:HOH:O	2.02	0.58
1:E:135:ASP:H	6:E:402:EDO:H11	1.68	0.56
1:H:186:ASP:OD2	1:H:188:VAL:HB	2.04	0.56
1:D:129:LEU:HB2	1:D:199:TYR:CE1	2.39	0.56
1:A:130:VAL:O	1:A:153:ILE:HA	2.05	0.56
1:D:240:GLU:O	1:D:280:GLY:N	2.38	0.56
1:E:136:GLY:N	6:E:402:EDO:H11	2.19	0.56
1:C:161:VAL:HG12	1:C:165:LYS:HE2	1.88	0.56
1:F:206:SER:O	3:F:402:PEG:H12	2.06	0.56
1:H:139:LEU:HD11	1:H:153:ILE:CD1	2.36	0.55
1:D:49:PRO:O	1:D:51:TRP:HD1	1.89	0.55
1:E:300:ILE:CD1	1:E:313:LEU:HD11	2.36	0.55
1:F:201:ALA:HA	1:F:234:VAL:O	2.07	0.55
1:E:300:ILE:HD13	1:E:313:LEU:HD11	1.89	0.55
1:C:166:GLN:HG2	1:C:167:TYR:CE2	2.41	0.54
1:A:191:LEU:HD21	1:A:225:VAL:HG22	1.89	0.54
1:E:135:ASP:N	6:E:402:EDO:C1	2.71	0.54
1:B:297:VAL:HG23	1:B:298:SER:N	2.22	0.54
1:D:191:LEU:HD21	1:D:225:VAL:HG22	1.90	0.54
1:D:131:ILE:HD11	1:D:191:LEU:HD22	1.90	0.54
1:A:333:LYS:HG3	1:A:334:VAL:N	2.24	0.53
1:F:266:TYR:OH	1:F:280:GLY:HA3	2.08	0.53
1:E:201:ALA:HA	1:E:234:VAL:O	2.09	0.53
1:F:45:SER:HB3	1:F:49:PRO:HA	1.91	0.53
1:H:248:ILE:O	1:H:252:ILE:HG13	2.09	0.53
1:D:96:LEU:HG	1:D:101:GLN:HG3	1.91	0.52
1:F:240:GLU:HB3	1:F:245[A]:HIS:ND1	2.25	0.52
1:E:138:VAL:N	6:E:402:EDO:C2	2.67	0.52
1:G:52:PHE:O	1:G:65:SER:HA	2.10	0.52
1:H:245:HIS:HB2	1:H:248:ILE:HG12	1.91	0.52
1:C:89:THR:HG21	1:D:60:PRO:O	2.09	0.52
1:H:245:HIS:CB	1:H:248:ILE:HG12	2.40	0.51
1:A:206:SER:O	3:A:402:PEG:H12	2.11	0.51
1:B:181:ASN:ND2	1:B:183:ILE:HD11	2.25	0.51
1:H:126:LYS:HD3	1:H:149:GLU:CD	2.35	0.51
1:A:237:THR:O	1:A:281:PHE:HA	2.10	0.51
1:G:297:VAL:HG23	1:G:298:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ALA:HA	1:C:234:VAL:O	2.11	0.51
1:F:64:HIS:HB3	7:F:640:HOH:O	2.10	0.51
1:E:209:PRO:O	1:E:214:LYS:HB2	2.11	0.50
1:E:127:LYS:HE2	1:E:198:THR:CG2	2.42	0.50
1:G:127:LYS:HE2	1:G:198:THR:CG2	2.41	0.50
1:F:107:GLU:OE1	1:F:135:ASP:OD2	2.30	0.50
1:C:130:VAL:O	1:C:153:ILE:HA	2.12	0.50
1:H:238:GLN:HG3	1:H:279:ILE:HG12	1.93	0.49
1:D:191:LEU:HD23	1:D:221:PHE:CE1	2.48	0.49
1:G:249:ILE:O	1:G:253:VAL:HG23	2.11	0.49
1:H:245:HIS:CB	1:H:248:ILE:CG1	2.88	0.49
1:A:126:LYS:NZ	7:A:505:HOH:O	2.45	0.49
1:F:231:PRO:HA	7:F:510:HOH:O	2.11	0.49
1:G:236:CYS:HA	1:G:282:MET:O	2.11	0.49
1:B:297:VAL:CG2	1:B:298:SER:N	2.76	0.49
1:D:201:ALA:HA	1:D:234:VAL:O	2.12	0.49
1:H:257:ARG:HD2	7:H:602:HOH:O	2.12	0.49
1:C:191:LEU:HD21	1:C:225:VAL:HG22	1.94	0.49
1:E:59:TRP:HB3	1:E:244:LEU:HD13	1.96	0.48
1:G:263:SER:O	1:G:284:CYS:HA	2.13	0.48
1:B:332:LYS:O	1:B:333:LYS:C	2.56	0.48
1:D:242:LEU:HD12	1:D:268:TRP:CE3	2.49	0.48
1:B:139:LEU:HD11	1:B:153:ILE:HD13	1.96	0.48
1:D:294:LYS:NZ	7:D:508:HOH:O	2.47	0.48
1:A:56:SER:HB3	1:A:59:TRP:CE2	2.48	0.48
1:D:183:ILE:HD13	1:D:190:PHE:CE1	2.49	0.48
1:G:140:ARG:HG3	1:G:140:ARG:HH11	1.79	0.47
1:F:52:PHE:O	1:F:65:SER:HA	2.14	0.47
1:D:130:VAL:O	1:D:153:ILE:HA	2.14	0.47
1:D:176:GLU:O	1:D:177:ASP:C	2.57	0.47
1:H:96:LEU:HD12	1:H:101:GLN:HG2	1.95	0.47
1:C:330:PHE:HA	1:C:333:LYS:HE3	1.97	0.47
1:C:330:PHE:O	1:C:333:LYS:HE3	2.15	0.47
1:B:292:ASP:OD2	1:D:292:ASP:OD2	2.32	0.47
1:D:127:LYS:HE3	1:D:150:GLN:OE1	2.14	0.47
1:D:236:CYS:HA	1:D:282:MET:O	2.13	0.47
1:E:319:GLU:HG3	7:E:620:HOH:O	2.15	0.47
1:G:208:ASP:OD1	3:G:401:PEG:H11	2.15	0.47
1:B:265:ASN:ND2	7:B:510:HOH:O	2.47	0.47
1:D:297:VAL:HG23	1:D:298:SER:HB3	1.96	0.47
1:E:138:VAL:HB	6:E:402:EDO:H21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:SER:O	1:E:333:LYS:HG3	2.15	0.46
1:F:67:LYS:NZ	7:F:512:HOH:O	2.47	0.46
1:H:142:VAL:O	1:H:145:HIS:HB2	2.15	0.46
1:B:124:ASN:N	1:B:125:PRO:CD	2.78	0.46
1:E:208:ASP:OD1	1:E:240:GLU:OE2	2.32	0.46
7:E:586:HOH:O	1:H:295:LYS:HE3	2.14	0.46
1:F:176:GLU:HA	1:F:176:GLU:OE1	2.16	0.46
1:G:57:PRO:O	1:G:60:PRO:HD3	2.16	0.46
1:A:201:ALA:HA	1:A:234:VAL:O	2.15	0.46
1:D:135:ASP:HA	1:D:164:ALA:HB1	1.96	0.46
1:E:274:TYR:OH	3:E:404:PEG:H42	2.15	0.46
1:A:153:ILE:C	1:A:153:ILE:HD13	2.41	0.46
1:E:127:LYS:NZ	1:E:198:THR:CG2	2.79	0.46
1:H:249:ILE:HD13	1:H:327:LEU:HD13	1.97	0.46
1:E:297:VAL:HG12	1:G:295:LYS:HE2	1.97	0.45
1:B:236:CYS:HA	1:B:282:MET:O	2.17	0.45
1:D:54:GLU:C	1:D:55:ILE:HD12	2.42	0.45
1:E:181:ASN:ND2	1:E:183:ILE:HD11	2.32	0.45
1:G:219:LYS:HB2	1:G:220:PRO:HD3	1.97	0.45
1:H:259:ILE:HD13	1:H:259:ILE:N	2.31	0.45
1:D:177:ASP:OD1	1:D:179:ARG:HB2	2.16	0.45
1:G:130:VAL:O	1:G:153:ILE:HA	2.16	0.45
1:D:237:THR:OG1	1:D:282:MET:HB2	2.17	0.45
1:E:133:GLY:HA2	1:E:153:ILE:HD11	1.97	0.45
1:E:127:LYS:NZ	7:E:509:HOH:O	2.49	0.45
1:H:82:VAL:HG11	1:H:163:VAL:HG21	1.99	0.45
1:A:49:PRO:HD3	1:B:47:ILE:HD13	1.98	0.45
1:H:214:LYS:HE3	7:H:606:HOH:O	2.17	0.44
1:C:139:LEU:HD11	1:C:153:ILE:HD13	1.99	0.44
1:E:58[A]:MET:SD	1:E:210:ILE:CG1	2.95	0.44
1:G:201:ALA:HA	1:G:234:VAL:O	2.18	0.44
1:C:155:GLU:O	1:C:184:ILE:HA	2.18	0.44
1:D:124:ASN:N	1:D:125:PRO:CD	2.81	0.44
1:E:195:ALA:O	1:E:198:THR:OG1	2.26	0.44
1:E:295:LYS:HE2	1:G:297:VAL:HG12	1.99	0.44
1:E:297:VAL:HG23	1:E:298:SER:HB3	1.99	0.43
1:C:182:LEU:HD21	1:C:184:ILE:HD11	1.99	0.43
1:E:135:ASP:HA	1:E:164:ALA:HB1	1.99	0.43
1:G:211:GLY:HA3	1:G:212:PRO:HD3	1.92	0.43
1:A:208:ASP:O	1:A:210:ILE:N	2.50	0.43
1:C:240:GLU:HB3	1:C:245:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:CYS:HA	1:C:282:MET:O	2.19	0.43
1:A:263:SER:O	1:A:284:CYS:HA	2.18	0.43
1:E:138:VAL:CB	6:E:402:EDO:H21	2.49	0.43
1:E:246:MET:CE	1:E:334:VAL:HG11	2.46	0.43
1:A:111:GLN:CD	1:A:137:GLY:HA3	2.44	0.43
1:F:237:THR:O	1:F:281:PHE:HA	2.18	0.43
1:E:79:TYR:CE1	1:E:156:ILE:HD13	2.54	0.43
1:H:263:SER:O	1:H:284:CYS:HA	2.19	0.43
1:B:55:ILE:HD13	1:B:63:ALA:HB2	2.01	0.42
1:C:188:VAL:HB	7:C:501:HOH:O	2.19	0.42
1:D:242:LEU:HD21	1:D:266:TYR:CE1	2.53	0.42
1:D:133:GLY:CA	1:D:153:ILE:HD11	2.47	0.42
1:A:127:LYS:HE3	1:A:198:THR:CG2	2.49	0.42
1:A:235:VAL:CG1	1:A:284:CYS:HB2	2.48	0.42
1:E:261:LYS:HB2	1:E:287:GLU:HB2	2.02	0.42
1:H:238:GLN:HG3	1:H:279:ILE:CG1	2.50	0.42
1:A:102:LEU:HD12	1:A:102:LEU:C	2.44	0.42
1:D:56:SER:HB3	1:D:59:TRP:CE2	2.55	0.42
1:F:265:ASN:HD22	1:F:293:PHE:HD2	1.67	0.42
1:F:219:LYS:N	1:F:220:PRO:CD	2.83	0.42
1:F:265:ASN:ND2	7:F:514:HOH:O	2.53	0.42
1:H:201:ALA:HA	1:H:234:VAL:O	2.20	0.42
1:A:336:ASP:O	1:A:337:SER:CB	2.67	0.42
1:B:237:THR:O	1:B:281:PHE:HA	2.20	0.42
1:G:208:ASP:HB3	1:G:209:PRO:HD2	2.02	0.42
1:B:58:MET:SD	1:B:208:ASP:HB3	2.60	0.42
1:A:67:LYS:HE3	7:A:572:HOH:O	2.20	0.42
1:B:92:LYS:NZ	1:B:167:TYR:O	2.40	0.42
1:C:161:VAL:HG12	1:C:165:LYS:CE	2.49	0.41
1:D:204:VAL:CG2	1:D:237:THR:HG22	2.50	0.41
1:E:93:VAL:HG22	1:E:103:THR:HG22	2.01	0.41
1:E:102:LEU:C	1:E:102:LEU:HD12	2.44	0.41
1:E:138:VAL:HG23	6:E:402:EDO:H21	2.01	0.41
1:H:126:LYS:CD	1:H:149:GLU:CD	2.93	0.41
1:E:155:GLU:O	1:E:184:ILE:HA	2.19	0.41
1:F:210:ILE:HG22	7:F:516:HOH:O	2.21	0.41
1:C:214:LYS:NZ	1:C:218:GLU:OE2	2.54	0.41
1:G:127:LYS:HE3	1:G:150:GLN:HE22	1.76	0.41
1:B:58:MET:HE3	1:B:58:MET:HB2	1.98	0.41
1:F:249:ILE:O	1:F:253:VAL:HG23	2.20	0.41
1:G:44:MET:HE3	1:G:44:MET:HB3	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:ARG:NE	7:H:520:HOH:O	2.54	0.41
1:C:268:TRP:CZ2	1:C:328:PRO:HD3	2.56	0.41
1:D:263:SER:O	1:D:284:CYS:HA	2.21	0.41
1:D:168:PHE:N	1:D:169:PRO:CD	2.84	0.41
1:H:73:PHE:HB2	1:H:167:TYR:CZ	2.56	0.41
1:H:174:GLY:HA2	7:H:609:HOH:O	2.21	0.41
1:B:295:LYS:HE2	1:D:297:VAL:HG12	2.02	0.41
1:E:154[B]:CYS:SG	1:E:187:GLY:HA2	2.61	0.41
1:F:286:SER:HA	7:F:502:HOH:O	2.20	0.41
1:A:52:PHE:O	1:A:65:SER:HA	2.21	0.40
1:B:297:VAL:HG12	1:D:295:LYS:HE2	2.02	0.40
1:E:263:SER:O	1:E:284:CYS:HA	2.21	0.40
1:G:253:VAL:O	1:G:257:ARG:HG3	2.20	0.40
1:F:266:TYR:CZ	1:F:280:GLY:HA3	2.56	0.40
1:E:161:VAL:HG12	1:E:165:LYS:HD2	2.02	0.40
1:F:208:ASP:HB3	1:F:209:PRO:HD2	2.04	0.40
1:E:127:LYS:NZ	1:E:198:THR:HG23	2.37	0.40

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	A	279/305 (92%)	254 (91%)	25 (9%)	0	100	100
1	B	284/305 (93%)	270 (95%)	14 (5%)	0	100	100
1	C	271/305 (89%)	259 (96%)	12 (4%)	0	100	100
1	D	269/305 (88%)	257 (96%)	12 (4%)	0	100	100
1	E	280/305 (92%)	273 (98%)	7 (2%)	0	100	100
1	F	285/305 (93%)	270 (95%)	15 (5%)	0	100	100
1	G	284/305 (93%)	270 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	278/305 (91%)	266 (96%)	12 (4%)	0	100	100
All	All	2230/2440 (91%)	2119 (95%)	111 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	247/264 (94%)	238 (96%)	9 (4%)	31	31
1	B	252/264 (96%)	247 (98%)	5 (2%)	48	54
1	C	239/264 (90%)	232 (97%)	7 (3%)	37	40
1	D	237/264 (90%)	229 (97%)	8 (3%)	32	33
1	E	245/264 (93%)	239 (98%)	6 (2%)	43	47
1	F	250/264 (95%)	245 (98%)	5 (2%)	48	54
1	G	249/264 (94%)	247 (99%)	2 (1%)	73	80
1	H	243/264 (92%)	238 (98%)	5 (2%)	47	52
All	All	1962/2112 (93%)	1915 (98%)	47 (2%)	43	47

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	71	ILE
1	A	153	ILE
1	A	163	VAL
1	A	176	GLU
1	A	191	LEU
1	A	279	ILE
1	A	311	CYS
1	A	320	ILE
1	B	163	VAL

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Mol	Chain	Res	Type
1	B	166	GLN
1	B	227	ARG
1	B	254	SER
1	B	305	SER
1	C	65	SER
1	C	123	SER
1	C	163	VAL
1	C	191	LEU
1	C	192	LYS
1	C	224	SER
1	C	238	GLN
1	D	49	PRO
1	D	70	LYS
1	D	191	LEU
1	D	238	GLN
1	D	269	THR
1	D	311	CYS
1	D	335	ILE
1	D	336	ASP
1	E	156	ILE
1	E	191	LEU
1	E	192	LYS
1	E	218	GLU
1	E	297	VAL
1	E	300	ILE
1	F	42	SER
1	F	126	LYS
1	F	127	LYS
1	F	131	ILE
1	F	238	GLN
1	G	300	ILE
1	G	320	ILE
1	H	101	GLN
1	H	156	ILE
1	H	207	SER
1	H	248	ILE
1	H	269	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN

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Mol	Chain	Res	Type
1	B	150	GLN
1	B	170	ASN
1	B	181	ASN
1	B	226	ASN
1	B	265	ASN
1	B	310	HIS
1	C	170	ASN
1	C	226	ASN
1	C	265	ASN
1	D	74	GLN
1	E	265	ASN
1	F	80	GLN
1	F	170	ASN
1	F	181	ASN
1	F	265	ASN
1	G	170	ASN
1	H	265	ASN

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](#)

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	PEG	D	404	-	6,6,6	0.22	0	5,5,5	0.15	0
2	ACT	H	402	-	3,3,3	1.07	0	3,3,3	0.75	0
2	ACT	A	401	-	3,3,3	0.99	0	3,3,3	0.84	0
4	FMT	E	406[A]	-	2,2,2	0.57	0	1,1,1	0.14	0
5	MLI	E	403	-	6,6,6	1.50	0	7,7,7	1.14	0
3	PEG	D	403	-	6,6,6	0.26	0	5,5,5	0.18	0
5	MLI	H	401	-	6,6,6	1.10	0	7,7,7	1.34	1 (14%)
4	FMT	B	402	-	2,2,2	0.28	0	1,1,1	0.21	0
4	FMT	E	405	-	2,2,2	0.19	0	1,1,1	0.20	0
3	PEG	C	401	-	6,6,6	0.31	0	5,5,5	0.21	0
5	MLI	D	401	-	6,6,6	1.77	2 (33%)	7,7,7	1.11	0
3	PEG	B	401	-	6,6,6	0.23	0	5,5,5	0.12	0
2	ACT	H	404	-	3,3,3	1.00	0	3,3,3	0.80	0
6	EDO	E	402	-	3,3,3	0.08	0	2,2,2	0.20	0
2	ACT	H	403	-	3,3,3	1.03	0	3,3,3	0.82	0
2	ACT	F	401	-	3,3,3	1.06	0	3,3,3	0.79	0
4	FMT	E	406[B]	-	2,2,2	0.05	0	1,1,1	0.15	0
3	PEG	F	403	-	6,6,6	0.21	0	5,5,5	0.30	0
5	MLI	E	401	-	6,6,6	1.87	2 (33%)	7,7,7	1.31	1 (14%)
3	PEG	A	402	-	6,6,6	0.14	0	5,5,5	0.13	0
3	PEG	D	402	-	6,6,6	0.21	0	5,5,5	0.18	0
3	PEG	E	404	-	6,6,6	0.47	0	5,5,5	0.40	0
3	PEG	F	402	-	6,6,6	0.24	0	5,5,5	0.18	0
3	PEG	G	401	-	6,6,6	0.45	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	C	401	-	-	2/4/4/4	-
5	MLI	D	401	-	-	4/4/4/4	-
3	PEG	D	403	-	-	3/4/4/4	-
5	MLI	E	401	-	-	2/4/4/4	-
3	PEG	B	401	-	-	2/4/4/4	-
3	PEG	A	402	-	-	2/4/4/4	-
5	MLI	E	403	-	-	4/4/4/4	-
3	PEG	D	404	-	-	3/4/4/4	-
6	EDO	E	402	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLI	H	401	-	-	4/4/4/4	-
3	PEG	D	402	-	-	3/4/4/4	-
3	PEG	E	404	-	-	0/4/4/4	-
3	PEG	F	402	-	-	1/4/4/4	-
3	PEG	G	401	-	-	0/4/4/4	-
3	PEG	F	403	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	401	MLI	O6-C2	3.69	1.34	1.22
5	D	401	MLI	O6-C2	3.11	1.32	1.22
5	D	401	MLI	O9-C3	-2.83	1.21	1.30
5	E	401	MLI	O8-C3	2.05	1.28	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	401	MLI	C3-C1-C2	2.50	121.77	112.95
5	H	401	MLI	O6-C2-C1	-2.14	116.02	122.11

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	PEG	O1-C1-C2-O2
3	C	401	PEG	O2-C3-C4-O4
3	F	403	PEG	O1-C1-C2-O2
3	B	401	PEG	O2-C3-C4-O4
3	D	403	PEG	O1-C1-C2-O2
3	A	402	PEG	O1-C1-C2-O2
3	D	404	PEG	O1-C1-C2-O2
5	D	401	MLI	C2-C1-C3-O9
5	E	401	MLI	C3-C1-C2-O6
3	B	401	PEG	C4-C3-O2-C2
5	D	401	MLI	C2-C1-C3-O8
3	A	402	PEG	O2-C3-C4-O4
5	E	403	MLI	C3-C1-C2-O6
5	E	403	MLI	C3-C1-C2-O7
3	D	402	PEG	C1-C2-O2-C3
5	E	403	MLI	C2-C1-C3-O8

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Mol	Chain	Res	Type	Atoms
3	D	404	PEG	C1-C2-O2-C3
5	E	401	MLI	C3-C1-C2-O7
5	H	401	MLI	C2-C1-C3-O8
5	H	401	MLI	C2-C1-C3-O9
3	D	403	PEG	C4-C3-O2-C2
5	E	403	MLI	C2-C1-C3-O9
3	D	404	PEG	C4-C3-O2-C2
3	F	402	PEG	O1-C1-C2-O2
5	H	401	MLI	C3-C1-C2-O7
5	D	401	MLI	C3-C1-C2-O6
3	C	401	PEG	O1-C1-C2-O2
3	D	403	PEG	O2-C3-C4-O4
5	D	401	MLI	C3-C1-C2-O7
5	H	401	MLI	C3-C1-C2-O6
3	D	402	PEG	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	402	EDO	17	0
3	F	403	PEG	1	0
3	A	402	PEG	1	0
3	E	404	PEG	1	0
3	F	402	PEG	1	0
3	G	401	PEG	1	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	284/305 (93%)	0.20	6 (2%) 63 63	21, 42, 64, 90	1 (0%)
1	B	290/305 (95%)	0.08	9 (3%) 51 50	21, 38, 64, 82	0
1	C	277/305 (90%)	0.23	7 (2%) 58 58	21, 42, 71, 87	0
1	D	275/305 (90%)	0.50	23 (8%) 17 15	25, 47, 83, 109	0
1	E	281/305 (92%)	-0.41	6 (2%) 63 63	11, 20, 43, 69	3 (1%)
1	F	287/305 (94%)	-0.16	6 (2%) 63 63	11, 27, 57, 89	2 (0%)
1	G	288/305 (94%)	-0.10	9 (3%) 51 50	13, 32, 56, 103	0
1	H	281/305 (92%)	0.09	4 (1%) 73 73	14, 35, 59, 80	1 (0%)
All	All	2263/2440 (92%)	0.05	70 (3%) 51 50	11, 36, 69, 109	7 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	299	LEU	5.4
1	G	212	PRO	4.5
1	H	44	MET	4.0
1	C	209	PRO	3.8
1	C	49	PRO	3.5
1	G	211	GLY	3.4
1	E	211	GLY	3.3
1	F	210	ILE	3.3
1	H	248	ILE	3.3
1	F	41	PRO	3.3
1	B	46	SER	3.2
1	D	49	PRO	3.2
1	B	213	ALA	3.1
1	A	193	ASN	3.1
1	B	210	ILE	3.0
1	B	299	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	300	ILE	3.0
1	G	299	LEU	2.9
1	D	50	GLY	2.9
1	A	337	SER	2.9
1	D	298	SER	2.9
1	A	43	CYS	2.8
1	G	210	ILE	2.8
1	B	337	SER	2.8
1	A	210	ILE	2.8
1	F	213	ALA	2.7
1	D	209	PRO	2.7
1	B	300	ILE	2.6
1	F	217	PHE	2.6
1	B	298	SER	2.5
1	G	300	ILE	2.5
1	D	55	ILE	2.5
1	D	71	ILE	2.5
1	D	57	PRO	2.5
1	C	301	ASP	2.4
1	D	82	VAL	2.4
1	E	213	ALA	2.4
1	D	335	ILE	2.4
1	G	335	ILE	2.4
1	D	64	HIS	2.4
1	G	298	SER	2.3
1	C	50	GLY	2.3
1	D	216	LEU	2.3
1	D	207	SER	2.3
1	G	337	SER	2.3
1	D	58	MET	2.3
1	B	47	ILE	2.3
1	E	133	GLY	2.3
1	E	210	ILE	2.2
1	F	212	PRO	2.2
1	D	70	LYS	2.2
1	D	214	LYS	2.2
1	E	300	ILE	2.2
1	H	249	ILE	2.2
1	D	79	TYR	2.2
1	F	337	SER	2.2
1	H	245	HIS	2.2
1	G	191	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	333	LYS	2.2
1	D	51	TRP	2.2
1	B	85	PHE	2.1
1	C	58	MET	2.1
1	C	71	ILE	2.1
1	C	83	ILE	2.1
1	D	63	ALA	2.1
1	A	335	ILE	2.1
1	D	73	PHE	2.1
1	D	163	VAL	2.1
1	A	188	VAL	2.0
1	D	169	PRO	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
2	ACT	H	402	4/4	0.63	0.20	48,49,52,54	0
4	FMT	B	402	3/3	0.77	0.20	67,67,68,69	0
4	FMT	E	405	3/3	0.77	0.14	49,49,51,54	0
2	ACT	A	401	4/4	0.83	0.15	30,30,33,36	4
5	MLI	D	401	7/7	0.83	0.15	41,42,43,44	7
5	MLI	E	401	7/7	0.83	0.13	26,28,30,32	7
2	ACT	F	401	4/4	0.86	0.11	21,24,25,30	4
3	PEG	D	404	7/7	0.86	0.14	25,27,37,39	7
3	PEG	C	401	7/7	0.87	0.14	50,53,56,57	0
3	PEG	F	403	7/7	0.87	0.12	36,38,43,46	7
3	PEG	D	403	7/7	0.87	0.11	46,53,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	H	403	4/4	0.88	0.14	26,26,28,32	4
6	EDO	E	402	4/4	0.88	0.14	21,21,21,23	4
2	ACT	H	404	4/4	0.90	0.12	25,32,33,38	4
3	PEG	D	402	7/7	0.90	0.13	55,57,61,63	0
5	MLI	E	403	7/7	0.91	0.09	27,35,38,39	7
5	MLI	H	401	7/7	0.91	0.11	32,37,40,43	7
3	PEG	A	402	7/7	0.91	0.12	48,56,57,59	0
3	PEG	B	401	7/7	0.94	0.10	44,47,51,51	0
3	PEG	F	402	7/7	0.94	0.07	28,30,37,39	0
4	FMT	E	406[B]	3/3	0.95	0.15	13,13,14,15	3
3	PEG	G	401	7/7	0.95	0.09	17,23,25,26	0
4	FMT	E	406[A]	3/3	0.95	0.15	7,7,7,7	3
3	PEG	E	404	7/7	0.97	0.06	12,13,16,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.