



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2017 – 01:33 PM EDT

PDB ID : 5X8F
Title : Ternary complex structure of a double mutant I454RA456K of o-Succinylbenzoate CoA Synthetase (MenE) from Bacillus Subtilis bound with AMP and its product analogue OSB-NCoA at 1.76 angstrom
Authors : Chen, Y.; Guo, Z.
Deposited on : unknown
Resolution : 1.76 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

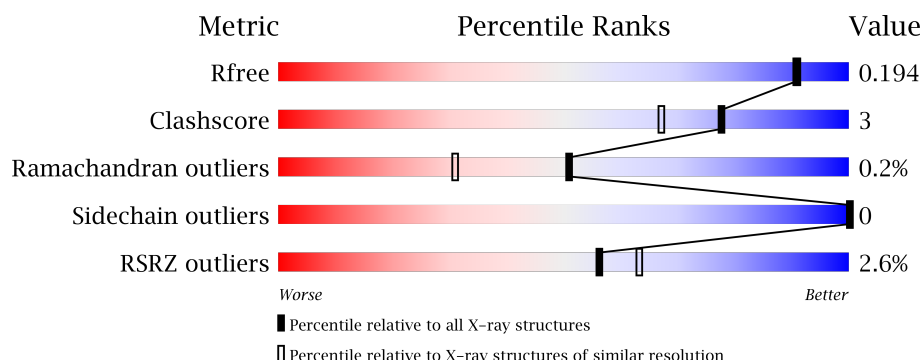
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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}	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	485	
1	B	485	
1	C	485	
1	D	485	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	A	502	-	-	-	X
3	AMP	C	502	-	-	-	X
4	MG	A	504	-	-	-	X
4	MG	B	508	-	-	-	X
5	NA	B	511	-	-	-	X
5	NA	B	513	-	-	-	X
5	NA	D	510	-	-	-	X
5	NA	D	515	-	-	-	X
6	PEG	A	517	-	-	-	X
6	PEG	B	520	-	-	-	X
6	PEG	C	515	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17221 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.

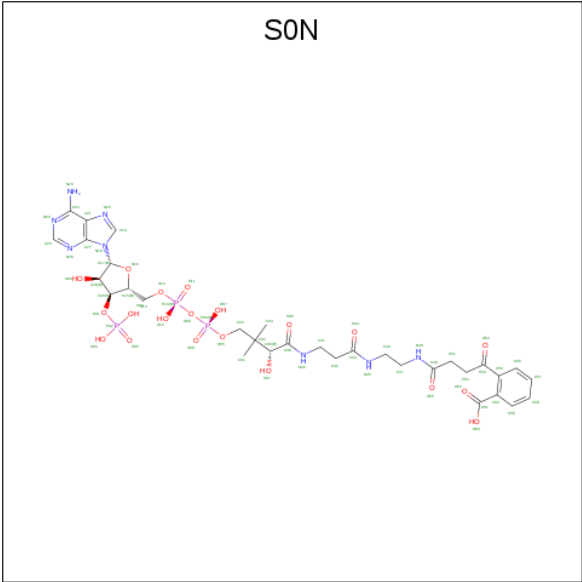
- Molecule 1 is a protein called 2-succinylbenzoate--CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	7	1
			3702	2363	615	701	23			
1	B	485	Total	C	N	O	S	0	4	0
			3678	2351	612	692	23			
1	C	485	Total	C	N	O	S	0	3	1
			3707	2365	626	693	23			
1	D	484	Total	C	N	O	S	0	6	0
			3692	2362	617	690	23			

There are 8 discrepancies between the modelled and reference sequences:

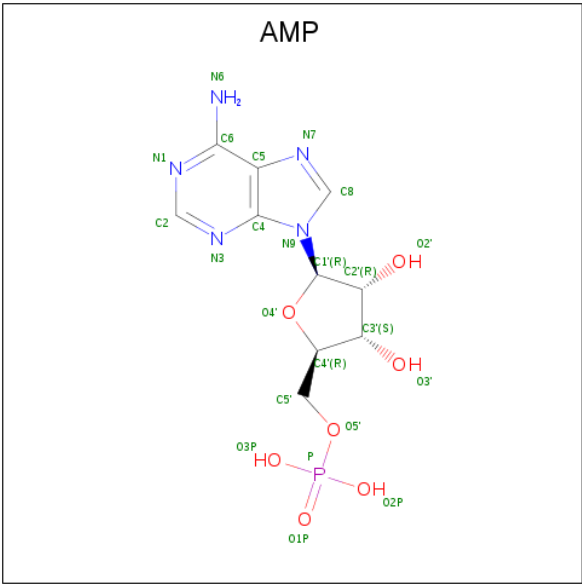
Chain	Residue	Modelled	Actual	Comment	Reference
A	454	ARG	ILE	engineered mutation	UNP P23971
A	456	LYS	ALA	engineered mutation	UNP P23971
B	454	ARG	ILE	engineered mutation	UNP P23971
B	456	LYS	ALA	engineered mutation	UNP P23971
C	454	ARG	ILE	engineered mutation	UNP P23971
C	456	LYS	ALA	engineered mutation	UNP P23971
D	454	ARG	ILE	engineered mutation	UNP P23971
D	456	LYS	ALA	engineered mutation	UNP P23971

- Molecule 2 is o-succinylbenzoyl-N-coenzyme A (three-letter code: S0N) (formula: $C_{32}H_{45}N_8O_{20}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	B	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	C	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	D	1	Total	C	N	O	P	0	0
			63	32	8	20	3		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total	Mg	0	0
			8	8		
4	A	8	Total	Mg	0	0
			8	8		
4	D	7	Total	Mg	0	0
			7	7		
4	C	4	Total	Mg	0	0
			4	4		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	9	Total	Na	0	0
			9	9		
5	A	5	Total	Na	0	0
			5	5		
5	D	11	Total	Na	0	0
			11	11		
5	C	8	Total	Na	0	0
			8	8		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

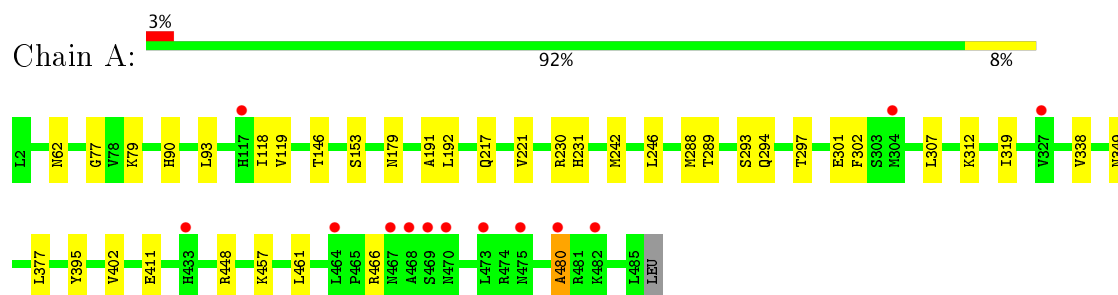
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	509	Total 509	O 509	0	0
8	B	496	Total 496	O 496	0	0
8	C	528	Total 528	O 528	0	0
8	D	499	Total 499	O 499	0	0

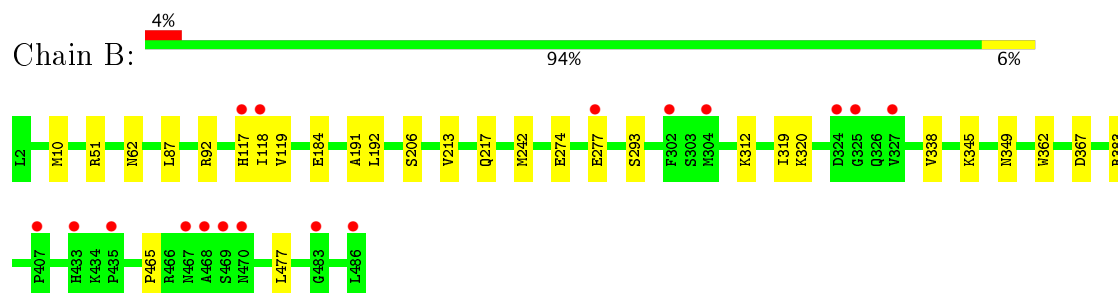
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

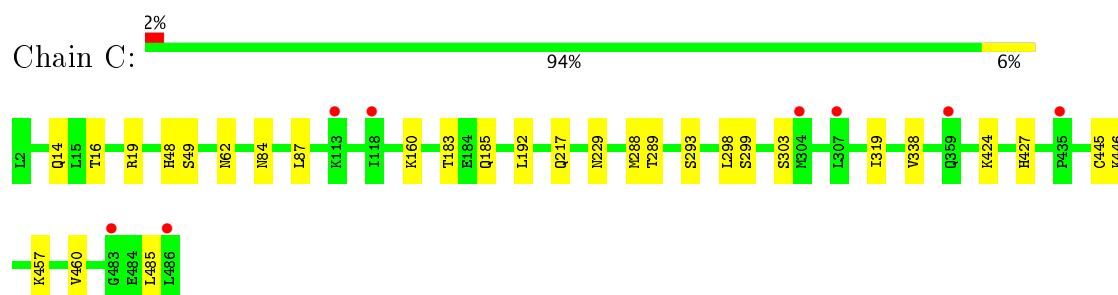
- Molecule 1: 2-succinylbenzoate--CoA ligase



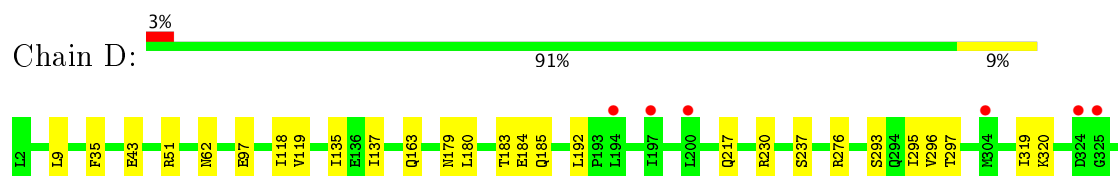
- Molecule 1: 2-succinylbenzoate--CoA ligase

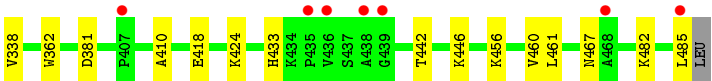


- Molecule 1: 2-succinylbenzoate--CoA ligase



- Molecule 1: 2-succinylbenzoate--CoA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.87Å 96.36Å 98.07Å 80.44° 77.96° 81.11°	Depositor
Resolution (Å)	29.96 – 1.76 29.96 – 1.76	Depositor EDS
% Data completeness (in resolution range)	92.9 (29.96-1.76) 88.6 (29.96-1.76)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.163 , 0.194 0.160 , 0.194	Depositor DCC
R_{free} test set	1984 reflections (0.86%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.049 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17221	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: MG, NA, CA, S0N, AMP, PEG

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	0.36	0/3794	0.57	1/5146 (0.0%)
1	B	0.37	0/3762	0.56	1/5106 (0.0%)
1	C	0.36	0/3785	0.53	0/5131
1	D	0.36	0/3785	0.57	1/5134 (0.0%)
All	All	0.36	0/15126	0.56	3/20517 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	B	191	ALA	C-N-CA	7.08	139.40	121.70
1	A	191	ALA	C-N-CA	6.46	137.84	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	ALA	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	A	3702	0	3608	29	0
1	B	3678	0	3588	19	0
1	C	3707	0	3635	21	0
1	D	3692	0	3628	28	0
2	A	63	0	40	2	0
2	B	63	0	40	2	0
2	C	63	0	40	0	0
2	D	63	0	40	0	0
3	A	23	0	12	4	0
3	C	23	0	12	2	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	C	4	0	0	0	0
4	D	7	0	0	0	0
5	A	5	0	0	0	0
5	B	9	0	0	0	0
5	C	8	0	0	0	0
5	D	11	0	0	0	0
6	A	14	0	20	0	0
6	B	14	0	20	4	0
6	C	14	0	20	1	0
6	D	7	0	10	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	509	0	0	9	1
8	B	496	0	0	4	0
8	C	528	0	0	6	0
8	D	499	0	0	10	1
All	All	17221	0	14713	100	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 3.

All (100) 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:C:445:CYS:SG	8:C:974:HOH:O	2.39	0.81
1:D:460:VAL:HG23	1:D:485:LEU:HD11	1.61	0.80
1:A:312:LYS:NZ	8:A:602:HOH:O	2.16	0.78
1:B:312:LYS:NZ	8:B:601:HOH:O	2.18	0.76
1:D:418:GLU:OE2	8:D:601:HOH:O	2.05	0.72
1:C:16:THR:HB	1:C:19:ARG:HG3	1.72	0.71
1:A:221:VAL:HG13	1:A:246:LEU:HD23	1.74	0.70
1:D:118:ILE:HG22	1:D:119:VAL:HG13	1.76	0.68
1:A:349[B]:ASN:OD1	1:B:349:ASN:ND2	2.26	0.68
1:C:319:ILE:HG22	1:C:338:VAL:HG12	1.76	0.68
1:B:319:ILE:HG22	1:B:338:VAL:HG12	1.76	0.67
1:A:77:GLY:O	8:A:601:HOH:O	2.12	0.67
1:D:163:GLN:NE2	8:D:608:HOH:O	2.28	0.66
1:D:456:LYS:NZ	8:D:605:HOH:O	2.24	0.66
1:C:229[B]:ASN:OD1	8:C:601:HOH:O	2.12	0.65
1:C:62:ASN:HB2	1:C:217:GLN:HA	1.82	0.62
3:A:502:AMP:N3	8:A:608:HOH:O	2.31	0.61
1:A:319[A]:ILE:HG22	1:A:338:VAL:HG12	1.82	0.61
1:A:79:LYS:NZ	8:A:610:HOH:O	2.33	0.60
1:A:457:LYS:NZ	8:A:611:HOH:O	2.34	0.60
1:D:184:GLU:O	8:D:602:HOH:O	2.17	0.59
6:B:520:PEG:H12	8:B:638:HOH:O	2.03	0.58
1:A:62:ASN:HB2	1:A:217:GLN:HA	1.87	0.57
1:C:424:LYS:NZ	8:C:619:HOH:O	2.38	0.56
1:A:230:ARG:HD3	1:A:231:HIS:CE1	2.41	0.56
1:A:79:LYS:HD2	1:A:146:THR:O	2.05	0.56
1:B:62:ASN:HB2	1:B:217:GLN:HA	1.88	0.55
1:C:14:GLN:HA	6:C:515:PEG:H12	1.89	0.55
1:A:179:ASN:OD1	1:A:297[B]:THR:HG21	2.08	0.54
1:C:192:LEU:HD12	1:C:192:LEU:O	2.09	0.52
1:D:424:LYS:NZ	8:D:617:HOH:O	2.41	0.52
1:D:442:THR:HG22	1:D:446:LYS:HE3	1.90	0.52
1:D:456:LYS:NZ	8:D:603:HOH:O	2.20	0.52
1:A:289:THR:N	3:A:502:AMP:O2P	2.40	0.52
1:D:62:ASN:HB2	1:D:217:GLN:HA	1.91	0.52
1:A:307:LEU:HD13	8:A:960:HOH:O	2.10	0.52
1:C:288:MET:HA	3:C:502:AMP:O3P	2.10	0.51
1:D:192:LEU:HD11	1:D:237:SER:O	2.11	0.51
1:B:345:LYS:HB2	6:B:520:PEG:H11	1.92	0.51
1:C:84:ASN:HB3	1:C:87:LEU:HG	1.92	0.51
1:D:179:ASN:OD1	1:D:297[B]:THR:HG21	2.11	0.51
1:B:51:ARG:NH1	8:B:610:HOH:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:OE1	1:D:118:ILE:HG23	2.11	0.50
1:D:43:GLU:HG2	1:D:135:ILE:HG12	1.93	0.50
3:A:502:AMP:O3'	8:A:603:HOH:O	2.20	0.50
1:A:192:LEU:CD2	2:A:501:S0N:H41	2.43	0.49
1:B:184:GLU:HG2	6:B:519:PEG:O2	2.13	0.49
1:C:48:HIS:O	1:C:49:SER:OG	2.25	0.48
1:A:192:LEU:HD21	1:A:242:MET:SD	2.53	0.47
1:A:294:GLN:OE1	1:A:297[A]:THR:HG21	2.15	0.47
1:D:381:ASP:OD2	8:D:604:HOH:O	2.20	0.47
1:C:192:LEU:HD12	1:C:192:LEU:C	2.35	0.47
1:C:460:VAL:HG23	1:C:485:LEU:HB2	1.97	0.47
1:D:276:ARG:NE	8:D:633:HOH:O	2.48	0.47
1:B:192:LEU:CD2	2:B:501:S0N:H41	2.46	0.47
1:D:410:ALA:HB2	1:D:433:HIS:CD2	2.50	0.46
1:A:402:VAL:HG13	1:A:448[A]:ARG:HD2	1.98	0.46
1:A:192:LEU:HD22	2:A:501:S0N:H41	1.96	0.46
6:B:519:PEG:H41	1:D:180:LEU:O	2.14	0.46
1:D:319[A]:ILE:HG22	1:D:338:VAL:HG12	1.97	0.46
1:A:301:GLU:HG3	1:A:302:PHE:CD2	2.51	0.45
1:C:427:HIS:CE1	1:C:457:LYS:HD2	2.51	0.45
1:C:289:THR:N	3:C:502:AMP:O3P	2.44	0.45
1:D:9:LEU:HD21	1:D:35:PHE:HA	1.97	0.45
1:A:118:ILE:HG22	1:A:119:VAL:HG13	1.99	0.45
1:D:320:LYS:HE2	1:D:362:TRP:CD2	2.52	0.45
1:A:461:LEU:HD21	1:A:480:ALA:O	2.16	0.44
1:A:288:MET:HA	3:A:502:AMP:O2P	2.17	0.44
1:B:274:GLU:HA	1:B:277:GLU:HG2	1.99	0.44
1:B:320:LYS:HE2	1:B:362:TRP:CD2	2.52	0.44
1:D:461:LEU:HG	1:D:482:LYS:HB3	1.99	0.44
1:B:117:HIS:CD2	1:B:118:ILE:HG12	2.53	0.44
1:C:183:THR:HG23	1:C:185:GLN:H	1.82	0.44
1:B:87:LEU:O	1:B:92:ARG:NH2	2.50	0.43
1:B:367:ASP:OD1	1:B:383:ARG:HD2	2.19	0.43
1:C:298:LEU:HD21	1:C:303:SER:HA	2.00	0.43
1:D:276:ARG:NE	8:D:634:HOH:O	2.51	0.43
1:D:295:ILE:HG23	1:D:296:VAL:HG23	2.01	0.43
1:A:192:LEU:HA	1:A:192:LEU:HD23	1.81	0.43
1:B:118:ILE:HG22	1:B:119:VAL:HG13	1.99	0.43
1:A:153[B]:SER:HA	1:A:395:TYR:CZ	2.55	0.42
1:C:446:LYS:HE3	1:C:446:LYS:HB2	1.77	0.42
1:A:217:GLN:NE2	8:A:622:HOH:O	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ASN:HB2	8:D:709:HOH:O	2.19	0.42
1:C:160:LYS:NZ	8:C:653:HOH:O	2.53	0.42
1:A:93:LEU:HD22	1:A:118:ILE:HD12	2.02	0.42
1:B:10:MET:HE1	8:B:852:HOH:O	2.19	0.41
1:C:229[B]:ASN:OD1	8:C:603:HOH:O	2.22	0.41
1:B:192:LEU:HD22	2:B:501:S0N:H41	2.02	0.41
1:D:230:ARG:HE	1:D:230:ARG:HB2	1.69	0.41
6:D:520:PEG:H12	6:D:520:PEG:H32	1.90	0.41
1:B:192:LEU:HD21	1:B:242:MET:SD	2.60	0.41
1:B:206:SER:HB2	1:B:213:VAL:HG23	2.02	0.41
1:D:183:THR:HG23	1:D:185:GLN:H	1.85	0.41
1:A:319[B]:ILE:CD1	1:A:377:LEU:HD22	2.50	0.41
1:A:411:GLU:OE1	1:A:466:ARG:NH2	2.50	0.41
1:A:90:HIS:HD2	8:A:643:HOH:O	2.02	0.41
1:B:465:PRO:HD2	1:B:477:LEU:HD23	2.02	0.41
1:D:137:ILE:HG13	1:D:137:ILE:H	1.63	0.41
1:C:299:SER:OG	8:C:602:HOH:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:622:HOH:O	8:D:683:HOH:O[1_556]	2.03	0.17

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	489/485 (101%)	478 (98%)	10 (2%)	1 (0%)	51	31
1	B	487/485 (100%)	477 (98%)	9 (2%)	1 (0%)	51	31
1	C	486/485 (100%)	478 (98%)	7 (1%)	1 (0%)	51	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	489/485 (101%)	479 (98%)	9 (2%)	1 (0%)	51	31
All	All	1951/1940 (101%)	1912 (98%)	35 (2%)	4 (0%)	51	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	SER
1	B	293	SER
1	C	293	SER
1	D	293	SER

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	385/414 (93%)	385 (100%)	0	100	100
1	B	383/414 (92%)	383 (100%)	0	100	100
1	C	387/414 (94%)	387 (100%)	0	100	100
1	D	386/414 (93%)	386 (100%)	0	100	100
All	All	1541/1656 (93%)	1541 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	393	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 76 ligands modelled in this entry, 63 are monoatomic - leaving 13 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	S0N	A	501	4	56,66,66	3.59	13 (23%)	66,97,97	1.93	10 (15%)
3	AMP	A	502	-	22,25,25	0.96	1 (4%)	24,38,38	1.67	2 (8%)
6	PEG	A	516	-	6,6,6	0.55	0	5,5,5	0.31	0
6	PEG	A	517	-	6,6,6	0.55	0	5,5,5	0.24	0
2	S0N	B	501	4	56,66,66	3.68	14 (25%)	66,97,97	1.94	11 (16%)
6	PEG	B	519	-	6,6,6	0.53	0	5,5,5	0.24	0
6	PEG	B	520	-	6,6,6	0.54	0	5,5,5	0.22	0
2	S0N	C	501	4	56,66,66	3.71	14 (25%)	66,97,97	1.83	9 (13%)
3	AMP	C	502	-	22,25,25	0.90	1 (4%)	24,38,38	1.75	4 (16%)
6	PEG	C	515	-	6,6,6	0.55	0	5,5,5	0.18	0
6	PEG	C	516	-	6,6,6	0.55	0	5,5,5	0.40	0
2	S0N	D	501	4	56,66,66	3.65	14 (25%)	66,97,97	1.99	11 (16%)
6	PEG	D	520	5	6,6,6	0.58	0	5,5,5	0.30	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	S0N	A	501	4	-	0/56/80/80	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	A	502	-	-	0/6/26/26	0/3/3/3
6	PEG	A	516	-	-	0/4/4/4	0/0/0/0
6	PEG	A	517	-	-	0/4/4/4	0/0/0/0
2	S0N	B	501	4	-	0/56/80/80	0/4/4/4
6	PEG	B	519	-	-	0/4/4/4	0/0/0/0
6	PEG	B	520	-	-	0/4/4/4	0/0/0/0
2	S0N	C	501	4	-	0/56/80/80	0/4/4/4
3	AMP	C	502	-	-	0/6/26/26	0/3/3/3
6	PEG	C	515	-	-	0/4/4/4	0/0/0/0
6	PEG	C	516	-	-	0/4/4/4	0/0/0/0
2	S0N	D	501	4	-	0/56/80/80	0/4/4/4
6	PEG	D	520	5	-	0/4/4/4	0/0/0/0

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	S0N	C28-C17	-16.24	1.27	1.53
2	B	501	S0N	C28-C17	-16.15	1.28	1.53
2	D	501	S0N	C28-C17	-15.97	1.28	1.53
2	A	501	S0N	C28-C17	-15.36	1.29	1.53
2	B	501	S0N	O16-C15	-7.13	1.28	1.45
2	A	501	S0N	O16-C15	-6.73	1.29	1.45
2	D	501	S0N	O16-C15	-6.66	1.29	1.45
2	C	501	S0N	O16-C15	-6.58	1.30	1.45
2	B	501	S0N	C21-C27	-3.38	1.32	1.40
2	A	501	S0N	C21-C27	-3.19	1.33	1.40
2	D	501	S0N	C21-C27	-3.10	1.33	1.40
2	C	501	S0N	C21-C27	-2.83	1.34	1.40
2	C	501	S0N	C01-C02	-2.12	1.49	1.53
2	B	501	S0N	C01-C02	-2.05	1.49	1.53
2	D	501	S0N	C59-C60	-2.04	1.36	1.39
2	A	501	S0N	C22-N23	2.06	1.42	1.34
2	B	501	S0N	C25-N26	2.26	1.36	1.32
2	B	501	S0N	C22-N23	2.32	1.43	1.34
2	C	501	S0N	C25-N26	2.35	1.36	1.32
2	A	501	S0N	C25-N26	2.35	1.36	1.32
2	C	501	S0N	C22-N23	2.37	1.43	1.34
2	D	501	S0N	C25-N26	2.41	1.36	1.32
2	D	501	S0N	C22-N23	2.49	1.44	1.34
3	C	502	AMP	C5-C4	3.06	1.47	1.40
2	B	501	S0N	C04-C02	3.13	1.56	1.52
3	A	502	AMP	C5-C4	3.19	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	S0N	C04-C02	3.22	1.57	1.52
2	C	501	S0N	O29-C28	3.52	1.51	1.43
2	A	501	S0N	O29-C28	3.54	1.51	1.43
2	D	501	S0N	O29-C28	3.61	1.51	1.43
2	A	501	S0N	C04-C02	3.62	1.57	1.52
2	B	501	S0N	O29-C28	3.62	1.51	1.43
2	D	501	S0N	C04-C02	3.64	1.57	1.52
2	A	501	S0N	C43-N45	3.91	1.42	1.33
2	B	501	S0N	C43-N45	4.12	1.43	1.33
2	D	501	S0N	C43-N45	4.18	1.43	1.33
2	A	501	S0N	C52-C53	4.21	1.57	1.51
2	C	501	S0N	C43-N45	4.23	1.43	1.33
2	B	501	S0N	C52-C53	4.25	1.57	1.51
2	D	501	S0N	C52-C53	4.32	1.57	1.51
2	A	501	S0N	C49-N48	4.54	1.44	1.33
2	D	501	S0N	C49-N48	4.66	1.44	1.33
2	C	501	S0N	C49-N48	4.70	1.44	1.33
2	B	501	S0N	C49-N48	4.89	1.44	1.33
2	C	501	S0N	C52-C53	4.97	1.58	1.51
2	B	501	S0N	C55-C53	5.20	1.59	1.48
2	D	501	S0N	C55-C53	5.25	1.59	1.48
2	A	501	S0N	C55-C53	5.40	1.59	1.48
2	D	501	S0N	C38-N40	5.46	1.44	1.33
2	C	501	S0N	C38-N40	5.58	1.45	1.33
2	B	501	S0N	C38-N40	5.62	1.45	1.33
2	C	501	S0N	C55-C53	5.78	1.60	1.48
2	A	501	S0N	C38-N40	6.00	1.45	1.33
2	A	501	S0N	O16-C17	15.44	1.62	1.41
2	B	501	S0N	O16-C17	15.61	1.62	1.41
2	D	501	S0N	O16-C17	15.75	1.63	1.41
2	C	501	S0N	O16-C17	15.95	1.63	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	S0N	N26-C25-N24	-10.31	119.88	128.86
2	B	501	S0N	N26-C25-N24	-10.06	120.10	128.86
2	A	501	S0N	N26-C25-N24	-9.93	120.21	128.86
2	C	501	S0N	N26-C25-N24	-9.55	120.54	128.86
3	C	502	AMP	N3-C2-N1	-6.38	123.31	128.86
2	C	501	S0N	C41-C42-C43	-5.88	102.77	112.22
3	A	502	AMP	N3-C2-N1	-5.78	123.82	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	S0N	C41-C42-C43	-5.71	103.04	112.22
2	B	501	S0N	C41-C42-C43	-5.53	103.33	112.22
2	B	501	S0N	C51-C52-C53	-4.96	105.98	112.66
2	D	501	S0N	C51-C52-C53	-4.89	106.06	112.66
2	C	501	S0N	C51-C52-C53	-4.42	106.70	112.66
2	A	501	S0N	C51-C52-C53	-4.14	107.08	112.66
2	A	501	S0N	C15-O16-C17	-4.05	105.45	109.77
2	A	501	S0N	C41-C42-C43	-3.94	105.88	112.22
2	A	501	S0N	O05-C04-C02	-3.76	104.50	110.55
3	A	502	AMP	C4-C5-N7	-3.73	105.81	109.41
2	D	501	S0N	O05-C04-C02	-3.00	105.72	110.55
3	C	502	AMP	C4-C5-N7	-2.69	106.81	109.41
2	B	501	S0N	O05-C04-C02	-2.59	106.39	110.55
2	B	501	S0N	C15-O16-C17	-2.56	107.05	109.77
2	B	501	S0N	O50-C49-N48	-2.49	118.22	122.97
2	C	501	S0N	C47-N48-C49	-2.44	118.17	122.84
2	A	501	S0N	O50-C49-N48	-2.40	118.40	122.97
2	B	501	S0N	C47-N48-C49	-2.36	118.31	122.84
2	D	501	S0N	C59-C60-C61	-2.35	116.62	120.23
2	C	501	S0N	O50-C49-N48	-2.33	118.53	122.97
2	C	501	S0N	C15-O16-C17	-2.32	107.30	109.77
3	C	502	AMP	O2P-P-O5'	-2.28	100.66	106.73
2	D	501	S0N	C47-N48-C49	-2.27	118.49	122.84
2	B	501	S0N	C41-N40-C38	-2.21	118.47	122.59
2	A	501	S0N	C46-N45-C43	-2.20	118.62	122.84
2	D	501	S0N	C52-C51-C49	-2.13	108.94	112.65
2	D	501	S0N	O50-C49-N48	-2.11	118.94	122.97
3	C	502	AMP	C2-N1-C6	2.08	122.41	118.77
2	D	501	S0N	C21-C22-N23	2.08	124.72	120.47
2	C	501	S0N	C21-C22-N23	2.13	124.81	120.47
2	A	501	S0N	C59-C60-C55	2.32	120.60	118.02
2	B	501	S0N	C21-C22-N23	2.36	125.28	120.47
2	B	501	S0N	C59-C60-C55	2.55	120.86	118.02
2	C	501	S0N	C01-C02-C36	2.64	113.41	108.82
2	C	501	S0N	C59-C60-C55	2.84	121.18	118.02
2	A	501	S0N	C01-C02-C36	2.85	113.77	108.82
2	D	501	S0N	C59-C60-C55	3.09	121.46	118.02
2	D	501	S0N	C01-C02-C36	3.39	114.70	108.82
2	B	501	S0N	C30-C28-C17	3.44	107.68	99.95
2	A	501	S0N	C30-C28-C17	3.97	108.86	99.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	S0N	2	0
3	A	502	AMP	4	0
2	B	501	S0N	2	0
6	B	519	PEG	2	0
6	B	520	PEG	2	0
3	C	502	AMP	2	0
6	C	515	PEG	1	0
6	D	520	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	484/485 (99%)	-0.05	13 (2%) 55 62	12, 24, 50, 85	0
1	B	485/485 (100%)	-0.02	17 (3%) 44 51	11, 23, 51, 69	0
1	C	485/485 (100%)	-0.20	8 (1%) 72 80	12, 25, 45, 64	0
1	D	484/485 (99%)	-0.10	13 (2%) 55 62	13, 26, 54, 87	0
All	All	1938/1940 (99%)	-0.09	51 (2%) 56 63	11, 25, 51, 87	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	ALA	7.2
1	C	486	LEU	4.9
1	B	468	ALA	4.8
1	A	469	SER	4.5
1	B	304	MET	4.5
1	D	435	PRO	3.9
1	B	325	GLY	3.8
1	B	435	PRO	3.8
1	A	470	ASN	3.4
1	A	467	ASN	3.4
1	D	324	ASP	3.4
1	B	118	ILE	3.3
1	D	436	VAL	3.2
1	C	118	ILE	3.0
1	D	438	ALA	3.0
1	D	485	LEU	3.0
1	B	470	ASN	3.0
1	B	327	VAL	3.0
1	A	327	VAL	3.0
1	B	117	HIS	2.9
1	A	482	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	480	ALA	2.8
1	D	468	ALA	2.7
1	B	467	ASN	2.7
1	A	473	LEU	2.7
1	B	486	LEU	2.7
1	A	433	HIS	2.7
1	D	407	PRO	2.6
1	C	307	LEU	2.6
1	B	324	ASP	2.6
1	D	304	MET	2.5
1	B	277	GLU	2.5
1	B	469	SER	2.5
1	B	302	PHE	2.5
1	C	304	MET	2.4
1	A	475	ASN	2.4
1	C	359	GLN	2.4
1	A	117	HIS	2.4
1	C	483	GLY	2.3
1	C	113	LYS	2.3
1	B	433	HIS	2.2
1	A	304	MET	2.1
1	B	407	PRO	2.1
1	A	464	LEU	2.1
1	D	200	LEU	2.1
1	D	194	LEU	2.1
1	D	197	ILE	2.1
1	B	483	GLY	2.0
1	C	435	PRO	2.0
1	D	325	GLY	2.0
1	D	439	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	504	1/1	0.97	0.17	22.56	39,39,39,39	0
3	AMP	A	502	23/23	0.65	0.35	15.09	25,37,58,62	23
5	NA	D	515	1/1	0.94	0.20	13.48	48,48,48,48	0
3	AMP	C	502	23/23	0.67	0.35	12.06	24,34,54,66	23
5	NA	B	511	1/1	0.88	0.23	10.59	64,64,64,64	0
5	NA	D	510	1/1	0.67	0.29	7.44	61,61,61,61	0
5	NA	B	513	1/1	0.62	0.17	5.70	58,58,58,58	0
6	PEG	C	515	7/7	0.83	0.18	4.18	38,53,66,67	0
6	PEG	A	517	7/7	0.94	0.09	3.42	33,39,48,54	0
6	PEG	B	520	7/7	0.86	0.20	3.02	31,40,65,68	0
4	MG	B	508	1/1	0.88	0.12	2.91	57,57,57,57	0
5	NA	B	515	1/1	0.89	0.14	1.75	52,52,52,52	0
4	MG	B	509	1/1	0.96	0.11	0.95	42,42,42,42	0
5	NA	C	512	1/1	0.82	0.19	0.92	62,62,62,62	0
6	PEG	B	519	7/7	0.87	0.12	0.77	30,37,44,47	0
4	MG	A	508	1/1	0.99	0.07	0.64	36,36,36,36	0
4	MG	C	506	1/1	0.94	0.12	0.60	37,37,37,37	0
5	NA	B	516	1/1	0.97	0.10	0.51	39,39,39,39	0
7	CA	A	518	1/1	1.00	0.09	0.43	34,34,34,34	0
2	S0N	C	501	63/63	0.90	0.10	0.42	13,22,51,55	0
2	S0N	D	501	63/63	0.91	0.11	0.24	10,21,46,51	0
7	CA	C	517	1/1	0.97	0.07	0.14	62,62,62,62	0
6	PEG	D	520	7/7	0.94	0.11	0.13	27,37,40,47	0
5	NA	D	512	1/1	0.85	0.09	-0.08	50,50,50,50	0
2	S0N	A	501	63/63	0.95	0.08	-0.30	13,20,32,36	0
5	NA	A	513	1/1	0.91	0.08	-0.32	46,46,46,46	0
2	S0N	B	501	63/63	0.94	0.09	-0.33	14,21,43,48	0
4	MG	A	505	1/1	0.90	0.10	-0.59	43,43,43,43	0
5	NA	D	514	1/1	0.97	0.07	-0.62	49,49,49,49	0
5	NA	A	512	1/1	0.96	0.05	-1.15	46,46,46,46	0
4	MG	A	509	1/1	0.96	0.07	-1.48	40,40,40,40	0
5	NA	B	510	1/1	0.98	0.06	-1.63	33,33,33,33	0
5	NA	D	519	1/1	0.85	0.08	-1.68	60,60,60,60	0
4	MG	B	504	1/1	1.00	0.05	-1.92	23,23,23,23	0
4	MG	D	503	1/1	0.99	0.04	-2.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	C	505	1/1	1.00	0.07	-2.12	22,22,22,22	0
4	MG	D	508	1/1	0.97	0.05	-2.68	33,33,33,33	0
4	MG	B	503	1/1	0.98	0.06	-2.85	32,32,32,32	0
4	MG	D	507	1/1	0.98	0.04	-3.26	37,37,37,37	0
4	MG	D	505	1/1	0.99	0.04	-5.10	23,23,23,23	0
4	MG	D	506	1/1	0.98	0.12	-	38,38,38,38	0
5	NA	C	514	1/1	0.96	0.14	-	48,48,48,48	0
5	NA	D	513	1/1	0.94	0.23	-	47,47,47,47	0
5	NA	C	509	1/1	0.87	0.10	-	53,53,53,53	0
4	MG	B	502	1/1	0.95	0.07	-	27,27,27,27	0
4	MG	D	504	1/1	0.93	0.05	-	36,36,36,36	0
4	MG	D	502	1/1	0.99	0.06	-	18,18,18,18	0
5	NA	C	513	1/1	0.54	0.24	-	73,73,73,73	0
5	NA	D	517	1/1	0.86	0.11	-	67,67,67,67	0
5	NA	C	510	1/1	0.88	0.10	-	50,50,50,50	0
4	MG	C	503	1/1	0.96	0.05	-	22,22,22,22	0
5	NA	C	511	1/1	0.89	0.06	-	59,59,59,59	0
4	MG	B	507	1/1	0.77	0.13	-	71,71,71,71	0
7	CA	B	521	1/1	0.87	0.09	-	64,64,64,64	0
4	MG	B	506	1/1	0.77	0.09	-	59,59,59,59	0
6	PEG	C	516	7/7	0.94	0.11	-	36,43,49,57	0
5	NA	B	512	1/1	0.97	0.10	-	38,38,38,38	0
4	MG	B	505	1/1	0.99	0.09	-	37,37,37,37	0
4	MG	A	503	1/1	0.99	0.05	-	22,22,22,22	0
5	NA	C	507	1/1	0.91	0.09	-	54,54,54,54	0
5	NA	B	518	1/1	0.95	0.10	-	52,52,52,52	0
5	NA	A	514	1/1	0.89	0.13	-	48,48,48,48	0
5	NA	B	514	1/1	0.82	0.24	-	70,70,70,70	0
5	NA	D	509	1/1	0.88	0.11	-	69,69,69,69	0
6	PEG	A	516	7/7	0.94	0.09	-	40,43,47,50	0
4	MG	C	504	1/1	0.84	0.05	-	65,65,65,65	0
5	NA	D	518	1/1	0.79	0.17	-	61,61,61,61	0
5	NA	D	511	1/1	0.89	0.10	-	62,62,62,62	0
4	MG	A	507	1/1	0.95	0.12	-	46,46,46,46	0
5	NA	D	516	1/1	0.84	0.14	-	69,69,69,69	0
5	NA	C	508	1/1	0.85	0.22	-	76,76,76,76	0
5	NA	B	517	1/1	0.90	0.16	-	40,40,40,40	0
5	NA	A	511	1/1	0.96	0.12	-	52,52,52,52	0
5	NA	A	515	1/1	0.92	0.09	-	60,60,60,60	0
4	MG	A	506	1/1	0.99	0.11	-	37,37,37,37	0
4	MG	A	510	1/1	0.93	0.20	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.