



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:35 AM GMT

PDB ID : 3P9I
Title : Crystal structure of perennial ryegrass LpOMT1 complexed with S-adenosyl-L-homocysteine and sinapaldehyde
Authors : Louie, G.V.; Noel, J.P.; Bowman, M.E.
Deposited on : 2010-10-17
Resolution : 1.85 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

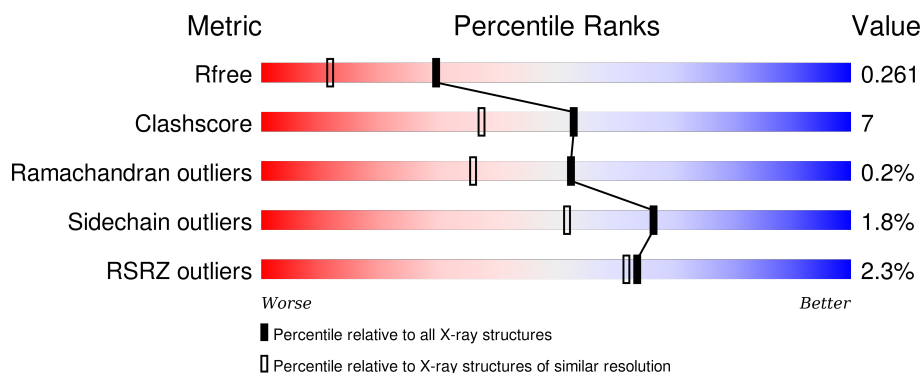
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	364	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	B	364	<div> <div>3%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	C	364	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	364	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>

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	BME	A	1089	-	-	-	X
4	BME	A	1295	-	-	-	X
4	BME	B	2089	-	-	-	X
4	BME	B	2295	-	-	X	X
4	BME	C	3089	-	-	-	X
4	BME	C	3295	-	-	-	X
4	BME	D	4089	-	-	-	X
4	BME	D	4295	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11726 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.

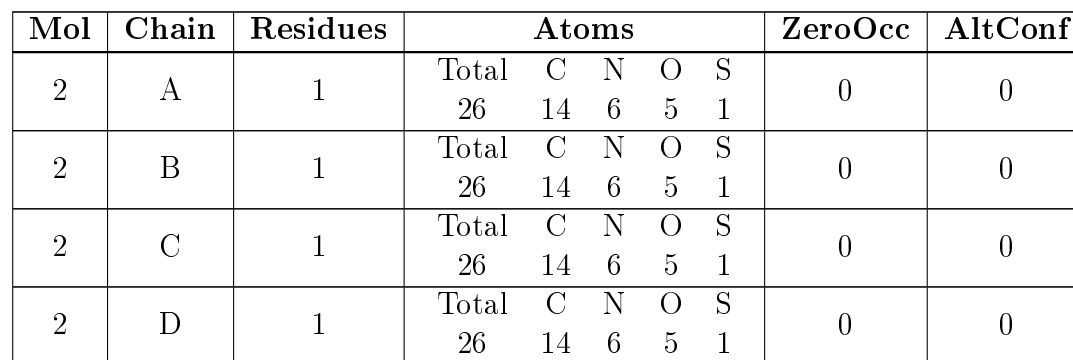
- Molecule 1 is a protein called Caffeic acid O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2704	1726	453	506	19			
1	B	356	Total	C	N	O	S	0	0	0
			2692	1719	451	503	19			
1	C	357	Total	C	N	O	S	0	0	0
			2698	1723	453	504	18			
1	D	351	Total	C	N	O	S	0	0	0
			2666	1704	447	497	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q9ZTU2
A	-2	SER	-	EXPRESSION TAG	UNP Q9ZTU2
A	-1	HIS	-	EXPRESSION TAG	UNP Q9ZTU2
A	0	GLY	-	EXPRESSION TAG	UNP Q9ZTU2
B	-3	GLY	-	EXPRESSION TAG	UNP Q9ZTU2
B	-2	SER	-	EXPRESSION TAG	UNP Q9ZTU2
B	-1	HIS	-	EXPRESSION TAG	UNP Q9ZTU2
B	0	GLY	-	EXPRESSION TAG	UNP Q9ZTU2
C	-3	GLY	-	EXPRESSION TAG	UNP Q9ZTU2
C	-2	SER	-	EXPRESSION TAG	UNP Q9ZTU2
C	-1	HIS	-	EXPRESSION TAG	UNP Q9ZTU2
C	0	GLY	-	EXPRESSION TAG	UNP Q9ZTU2
D	-3	GLY	-	EXPRESSION TAG	UNP Q9ZTU2
D	-2	SER	-	EXPRESSION TAG	UNP Q9ZTU2
D	-1	HIS	-	EXPRESSION TAG	UNP Q9ZTU2
D	0	GLY	-	EXPRESSION TAG	UNP Q9ZTU2

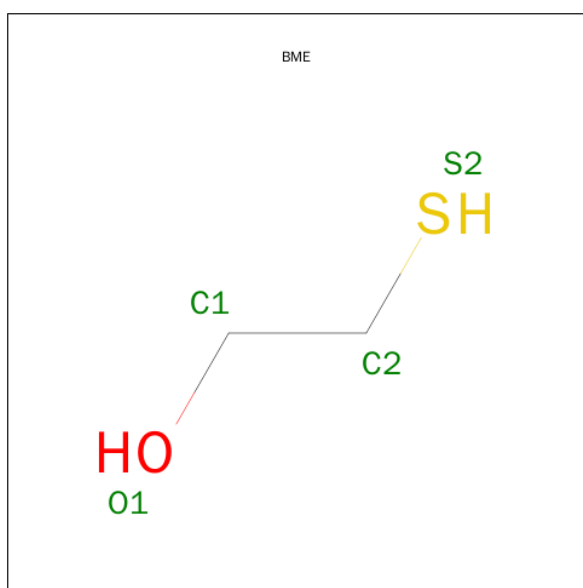
- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



- SNY
-
- Chemical structure of 3-methoxy-4-(3-methoxyphenyl)-2-propenoic acid (SNY). The structure shows a central benzene ring with a propenoic acid side chain at position 1, a methoxy group at position 3, and a 3-methoxyphenyl group at position 4. Atoms are labeled with green text: carbons C1-C9, oxygens O3-O5, and methyl groups C3M and C5M.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	11	4		
3	B	1	Total	C	O	0	0
			15	11	4		
3	C	1	Total	C	O	0	0
			15	11	4		
3	D	1	Total	C	O	0	0
			15	11	4		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



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

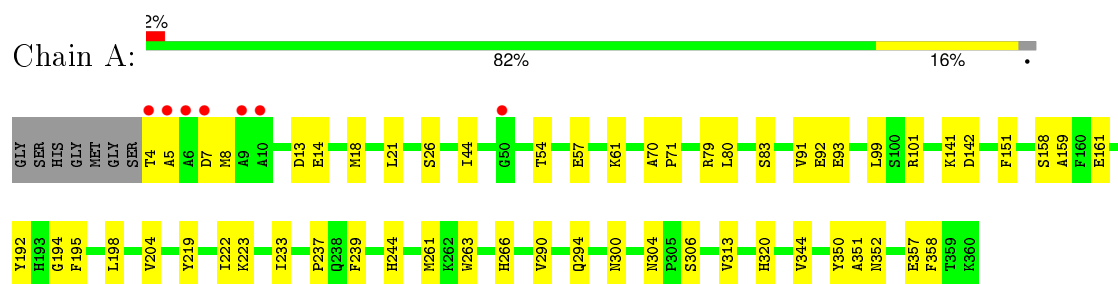
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	180	Total 180	O 180	0	0
5	B	181	Total 181	O 181	0	0
5	C	222	Total 222	O 222	0	0
5	D	187	Total 187	O 187	0	0

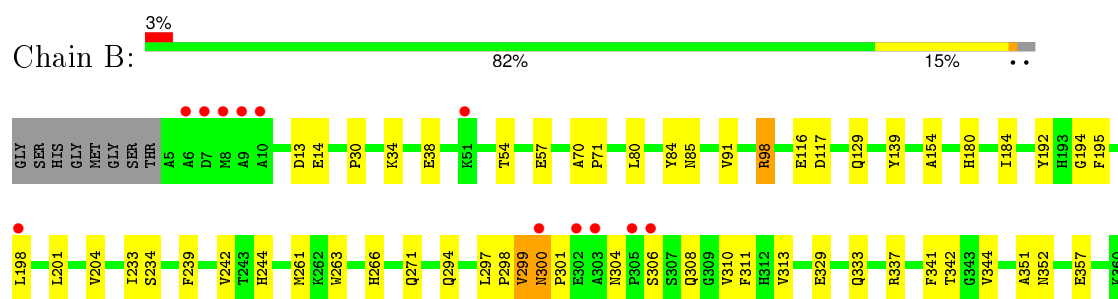
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

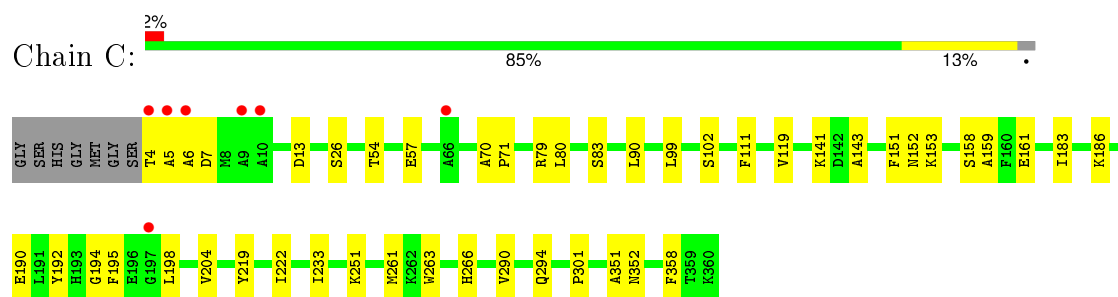
• Molecule 1: Caffeic acid O-methyltransferase



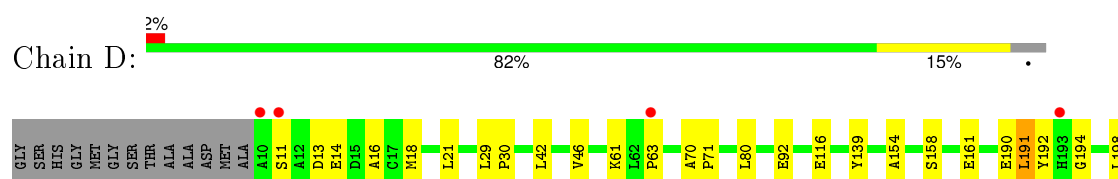
• Molecule 1: Caffeic acid O-methyltransferase

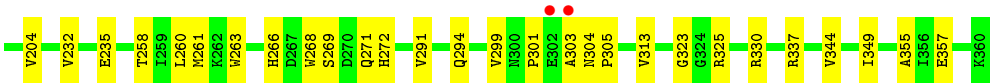


• Molecule 1: Caffeic acid O-methyltransferase



• Molecule 1: Caffeic acid O-methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.94Å 85.22Å 98.57Å 90.00° 111.10° 90.00°	Depositor
Resolution (Å)	47.07 – 1.85 47.07 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (47.07-1.85) 92.3 (47.07-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.261 0.232 , 0.261	Depositor DCC
R_{free} test set	5945 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.915	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.6	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	5 of 148516 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11726	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.66 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4778e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SAH, BME, SNY

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	0.33	0/2767	0.57	0/3759
1	B	0.33	0/2755	0.57	0/3742
1	C	0.34	0/2761	0.57	0/3752
1	D	0.34	0/2729	0.57	0/3707
All	All	0.34	0/11012	0.57	0/14960

There are no bond length outliers.

There are no bond angle outliers.

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	2704	0	2675	41	0
1	B	2692	0	2657	43	0
1	C	2698	0	2666	32	0
1	D	2666	0	2640	39	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	15	0	11	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	11	1	0
3	C	15	0	11	1	0
3	D	15	0	11	1	0
4	A	8	0	10	3	0
4	B	8	0	10	5	0
4	C	8	0	10	1	0
4	D	8	0	10	1	0
5	A	180	0	0	3	0
5	B	181	0	0	2	0
5	C	222	0	0	4	0
5	D	187	0	0	2	0
All	All	11726	0	10798	144	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 7.

All (144) 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:B:313:VAL:HG21	4:B:2295:BME:H22	1.46	0.96
1:C:4:THR:HG22	1:C:6:ALA:H	1.42	0.84
1:A:91:VAL:HG22	1:A:101:ARG:HG2	1.64	0.78
1:D:190:GLU:C	1:D:191:LEU:HD23	2.09	0.73
1:C:119:VAL:HG23	1:C:183:ILE:HD11	1.69	0.73
1:A:14:GLU:O	1:A:18:MET:HG3	1.90	0.72
1:C:99:LEU:HD11	1:D:299:VAL:HG13	1.72	0.72
1:C:4:THR:HB	1:C:7:ASP:CB	2.20	0.71
1:A:233:ILE:HG23	1:A:244:HIS:HB3	1.73	0.70
1:B:313:VAL:HG21	4:B:2295:BME:C2	2.23	0.68
1:C:251:LYS:HE2	5:C:1660:HOH:O	1.93	0.66
1:B:233:ILE:HG23	1:B:244:HIS:HB3	1.78	0.66
1:A:219:TYR:HB3	1:A:222:ILE:HD13	1.79	0.65
1:B:271:GLN:HG3	5:B:1237:HOH:O	1.98	0.64
1:C:186:LYS:O	1:C:190:GLU:HG3	1.97	0.64
1:C:79:ARG:HG3	4:C:3089:BME:H12	1.81	0.63
1:A:4:THR:HA	1:A:7:ASP:HB2	1.80	0.63
1:A:313:VAL:HG21	4:A:1295:BME:S2	2.40	0.61
1:D:116:GLU:H	1:D:116:GLU:CD	2.04	0.61
1:D:299:VAL:O	1:D:301:PRO:HD3	2.00	0.61
4:A:1089:BME:H11	5:A:1429:HOH:O	2.00	0.61
1:C:70:ALA:HB3	1:C:71:PRO:HD3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:HB	1:C:261:MET:HG2	1.83	0.60
1:D:61:LYS:O	1:D:63:PRO:HD3	2.02	0.60
1:D:80:LEU:C	1:D:80:LEU:HD13	2.22	0.59
1:D:191:LEU:HD23	1:D:191:LEU:N	2.17	0.59
1:A:4:THR:O	1:A:7:ASP:N	2.35	0.59
1:B:299:VAL:O	1:B:300:ASN:HB2	2.04	0.58
1:A:18:MET:SD	1:B:306:SER:HB2	2.43	0.58
1:B:139:TYR:CD2	1:B:154:ALA:HB2	2.39	0.57
1:A:158:SER:OG	1:A:161:GLU:HG3	2.04	0.57
1:A:101:ARG:HD2	4:A:1089:BME:S2	2.45	0.56
1:D:139:TYR:CD2	1:D:154:ALA:HB2	2.40	0.56
1:A:204:VAL:HB	1:A:261:MET:HG2	1.87	0.56
1:A:4:THR:O	1:A:8:MET:N	2.39	0.56
1:A:83:SER:HB2	1:B:308:GLN:HG2	1.87	0.56
1:C:158:SER:OG	1:C:161:GLU:HG3	2.06	0.56
1:C:4:THR:HB	1:C:7:ASP:H	1.72	0.55
1:D:14:GLU:O	1:D:18:MET:HG3	2.07	0.54
1:B:329:GLU:HG2	1:B:333:GLN:HE21	1.71	0.54
1:D:192:TYR:CZ	1:D:194:GLY:HA3	2.43	0.54
1:D:337:ARG:HG3	1:D:337:ARG:HH11	1.73	0.54
1:A:192:TYR:CZ	1:A:194:GLY:HA3	2.43	0.53
1:B:313:VAL:CG2	4:B:2295:BME:H22	2.29	0.53
1:A:4:THR:O	1:A:5:ALA:C	2.47	0.53
1:A:344:VAL:HA	1:A:357:GLU:O	2.09	0.53
1:B:263:TRP:O	3:B:602:SNY:H5M	2.09	0.53
1:B:70:ALA:HB3	1:B:71:PRO:HD3	1.90	0.52
1:A:195:PHE:HA	1:A:198:LEU:HD12	1.89	0.52
1:C:4:THR:HG22	1:C:5:ALA:N	2.25	0.52
1:B:91:VAL:HG13	4:B:2089:BME:S2	2.50	0.52
1:A:44:ILE:HG23	1:A:61:LYS:HD2	1.92	0.51
1:A:101:ARG:HD3	5:A:1429:HOH:O	2.10	0.51
1:D:263:TRP:O	3:D:604:SNY:H5M	2.10	0.51
1:A:54:THR:OG1	1:A:57:GLU:HG3	2.11	0.51
1:D:204:VAL:HB	1:D:261:MET:HG2	1.92	0.50
1:C:351:ALA:O	1:C:352:ASN:HB2	2.12	0.50
1:D:70:ALA:HB3	1:D:71:PRO:HD3	1.94	0.50
1:C:192:TYR:CZ	1:C:194:GLY:HA3	2.46	0.50
1:D:190:GLU:CB	1:D:191:LEU:HD23	2.42	0.50
1:C:26:SER:OG	1:D:30:PRO:HB3	2.12	0.50
1:A:151:PHE:CE2	1:A:159:ALA:HA	2.47	0.50
1:C:219:TYR:HB2	1:C:222:ILE:HD12	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:C	1:A:80:LEU:HD13	2.31	0.50
1:D:313:VAL:HG21	4:D:4295:BME:S2	2.52	0.49
1:B:34:LYS:HD2	1:B:129:GLN:HB3	1.93	0.49
1:B:34:LYS:O	1:B:38:GLU:HG3	2.12	0.49
1:D:304:ASN:HB2	1:D:305:PRO:HD2	1.94	0.49
1:B:180:HIS:CE1	1:B:184:ILE:HG13	2.48	0.49
1:C:90:LEU:HB3	1:C:102:SER:OG	2.12	0.49
1:B:98:ARG:HG3	1:B:98:ARG:HH11	1.78	0.49
1:A:304:ASN:OD1	1:A:306:SER:HB3	2.13	0.48
1:C:151:PHE:CE2	1:C:159:ALA:HA	2.48	0.48
1:D:260:LEU:HD12	1:D:291:VAL:O	2.14	0.47
1:D:42:LEU:O	1:D:46:VAL:HG23	2.14	0.47
1:B:80:LEU:HD13	1:B:80:LEU:C	2.34	0.47
1:A:141:LYS:HB3	1:A:141:LYS:NZ	2.29	0.47
1:B:298:PRO:C	1:B:300:ASN:H	2.18	0.47
1:A:263:TRP:O	3:A:601:SNY:H5M	2.14	0.47
1:B:344:VAL:HA	1:B:357:GLU:O	2.15	0.47
1:A:151:PHE:HB2	1:A:320:HIS:HA	1.96	0.47
1:A:4:THR:HB	1:A:8:MET:HG3	1.96	0.46
1:D:325:ARG:HD2	5:D:1111:HOH:O	2.14	0.46
1:A:70:ALA:HB3	1:A:71:PRO:HD3	1.98	0.46
1:D:158:SER:OG	1:D:161:GLU:HG3	2.15	0.46
1:C:111:PHE:HE2	1:D:16:ALA:HB3	1.79	0.46
1:C:351:ALA:HB1	1:D:21:LEU:CD1	2.46	0.46
1:D:299:VAL:C	1:D:301:PRO:HD3	2.36	0.46
1:A:237:PRO:HG2	1:A:239:PHE:CZ	2.51	0.45
1:A:91:VAL:HG11	1:A:99:LEU:HD13	1.97	0.45
1:A:290:VAL:HB	1:A:358:PHE:HB2	1.98	0.45
1:A:21:LEU:HD13	4:B:2295:BME:O1	2.16	0.45
1:D:232:VAL:O	1:D:235:GLU:HG2	2.17	0.45
1:A:350:TYR:CE1	1:B:14:GLU:HB2	2.51	0.45
1:B:342:THR:HG22	5:B:1781:HOH:O	2.16	0.45
1:B:116:GLU:HG2	1:B:117:ASP:N	2.32	0.45
5:C:1307:HOH:O	1:D:305:PRO:HG3	2.16	0.45
1:A:91:VAL:HG12	1:A:92:GLU:N	2.32	0.44
1:C:54:THR:OG1	1:C:57:GLU:HG3	2.17	0.44
1:B:54:THR:OG1	1:B:57:GLU:HG3	2.17	0.44
1:C:263:TRP:O	3:C:603:SNY:H5M	2.17	0.44
1:B:304:ASN:C	1:B:306:SER:H	2.21	0.44
1:C:152:ASN:HD22	1:C:152:ASN:N	2.15	0.44
1:D:198:LEU:HD21	1:D:258:THR:OG1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PHE:O	1:C:198:LEU:HB2	2.18	0.44
1:C:83:SER:O	1:D:303:ALA:HB1	2.18	0.44
1:A:44:ILE:HD13	1:A:61:LYS:HB2	2.00	0.44
1:B:299:VAL:O	1:B:300:ASN:CB	2.65	0.43
1:C:143:ALA:HA	1:C:153:LYS:HE3	2.01	0.43
1:B:198:LEU:HD13	1:B:201:LEU:HB2	2.01	0.43
1:D:29:LEU:HB3	1:D:30:PRO:CD	2.49	0.43
1:C:152:ASN:H	1:C:152:ASN:HD22	1.66	0.43
1:A:351:ALA:O	1:A:352:ASN:HB2	2.19	0.43
1:B:192:TYR:CZ	1:B:194:GLY:HA3	2.54	0.42
1:A:26:SER:OG	1:B:30:PRO:HB3	2.19	0.42
1:C:4:THR:HB	1:C:7:ASP:N	2.32	0.42
1:D:268:TRP:HB3	1:D:272:HIS:HB2	2.02	0.42
5:C:1307:HOH:O	1:D:305:PRO:CG	2.68	0.42
1:B:98:ARG:C	1:B:98:ARG:HD3	2.39	0.42
1:B:351:ALA:O	1:B:352:ASN:HB2	2.20	0.42
1:A:18:MET:HE2	1:B:352:ASN:ND2	2.35	0.42
1:C:195:PHE:HA	1:C:198:LEU:HD12	2.01	0.42
1:A:79:ARG:HD2	1:B:311:PHE:CE1	2.55	0.41
1:B:337:ARG:HD3	1:B:341:PHE:O	2.19	0.41
1:D:269:SER:HB3	1:D:323:GLY:HA3	2.01	0.41
1:C:141:LYS:CG	5:C:1123:HOH:O	2.67	0.41
1:D:349:ILE:HD11	1:D:355:ALA:HB2	2.01	0.41
1:D:271:GLN:H	1:D:271:GLN:CD	2.23	0.41
1:A:141:LYS:HB3	5:A:1400:HOH:O	2.21	0.41
1:B:195:PHE:O	1:B:198:LEU:HB2	2.21	0.41
1:B:84:TYR:O	1:B:85:ASN:HB2	2.19	0.41
1:C:290:VAL:HB	1:C:358:PHE:HB2	2.02	0.41
1:C:80:LEU:HD13	1:C:80:LEU:C	2.41	0.41
1:B:98:ARG:NH1	1:B:98:ARG:HG3	2.35	0.41
1:D:330:ARG:HG2	5:D:1651:HOH:O	2.20	0.41
1:B:239:PHE:HB2	1:B:242:VAL:HB	2.02	0.41
1:B:329:GLU:HG2	1:B:333:GLN:NE2	2.36	0.41
1:B:204:VAL:HB	1:B:261:MET:HG2	2.02	0.41
1:D:344:VAL:HA	1:D:357:GLU:O	2.21	0.41
1:B:297:LEU:HD23	1:B:310:VAL:HG11	2.03	0.40
1:A:222:ILE:C	1:A:223:LYS:HD2	2.41	0.40
1:D:337:ARG:CG	1:D:337:ARG:HH11	2.34	0.40
1:B:234:SER:HB3	1:D:11:SER:HB3	2.02	0.40
1:B:329:GLU:O	1:B:333:GLN:HG3	2.22	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	355/364 (98%)	347 (98%)	8 (2%)	0	100	100
1	B	354/364 (97%)	342 (97%)	9 (2%)	3 (1%)	24	9
1	C	355/364 (98%)	346 (98%)	9 (2%)	0	100	100
1	D	349/364 (96%)	339 (97%)	10 (3%)	0	100	100
All	All	1413/1456 (97%)	1374 (97%)	36 (2%)	3 (0%)	52	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	ASN
1	B	301	PRO
1	B	299	VAL

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	284/288 (99%)	278 (98%)	6 (2%)	61	45
1	B	281/288 (98%)	277 (99%)	4 (1%)	74	63
1	C	282/288 (98%)	277 (98%)	5 (2%)	66	52
1	D	281/288 (98%)	276 (98%)	5 (2%)	66	52
All	All	1128/1152 (98%)	1108 (98%)	20 (2%)	66	52

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	93	GLU
1	A	142	ASP
1	A	266	HIS
1	A	294	GLN
1	A	300	ASN
1	B	13	ASP
1	B	98	ARG
1	B	266	HIS
1	B	294	GLN
1	C	13	ASP
1	C	233	ILE
1	C	266	HIS
1	C	294	GLN
1	C	301	PRO
1	D	13	ASP
1	D	92	GLU
1	D	191	LEU
1	D	266	HIS
1	D	294	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	85	ASN
1	A	193	HIS
1	A	294	GLN
1	A	300	ASN
1	B	85	ASN
1	B	294	GLN
1	B	308	GLN
1	B	333	GLN
1	B	352	ASN
1	C	152	ASN
1	C	218	HIS
1	C	294	GLN
1	D	85	ASN
1	D	218	HIS
1	D	352	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 ⓘ

16 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$
4	BME	A	1089	1	3,3,3	0.16	0	2,2,2	0.40	0
4	BME	A	1295	1	3,3,3	0.25	0	2,2,2	0.45	0
2	SAH	A	401	-	20,28,28	1.04	2 (10%)	19,40,40	2.69	5 (26%)
3	SNY	A	601	-	15,15,15	3.01	4 (26%)	18,19,19	2.38	5 (27%)
4	BME	B	2089	1	3,3,3	0.24	0	2,2,2	0.43	0
4	BME	B	2295	1	3,3,3	0.25	0	2,2,2	0.27	0
2	SAH	B	402	-	20,28,28	1.10	2 (10%)	19,40,40	2.67	5 (26%)
3	SNY	B	602	-	15,15,15	2.98	4 (26%)	18,19,19	2.40	6 (33%)
4	BME	C	3089	1	3,3,3	0.20	0	2,2,2	0.43	0
4	BME	C	3295	1	3,3,3	0.31	0	2,2,2	0.35	0
2	SAH	C	403	-	20,28,28	0.91	2 (10%)	19,40,40	2.64	3 (15%)
3	SNY	C	603	-	15,15,15	2.97	4 (26%)	18,19,19	2.36	5 (27%)
2	SAH	D	404	-	20,28,28	1.00	1 (5%)	19,40,40	2.60	3 (15%)
4	BME	D	4089	1	3,3,3	0.25	0	2,2,2	0.45	0
4	BME	D	4295	1	3,3,3	0.25	0	2,2,2	0.45	0
3	SNY	D	604	-	15,15,15	2.97	4 (26%)	18,19,19	2.38	6 (33%)

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
4	BME	A	1089	1	-	0/1/1/1	0/0/0/0
4	BME	A	1295	1	-	0/1/1/1	0/0/0/0
2	SAH	A	401	-	-	0/7/31/31	0/3/3/3
3	SNY	A	601	-	-	0/8/8/8	0/1/1/1
4	BME	B	2089	1	-	0/1/1/1	0/0/0/0
4	BME	B	2295	1	-	0/1/1/1	0/0/0/0
2	SAH	B	402	-	-	0/7/31/31	0/3/3/3
3	SNY	B	602	-	-	0/8/8/8	0/1/1/1
4	BME	C	3089	1	-	0/1/1/1	0/0/0/0
4	BME	C	3295	1	-	0/1/1/1	0/0/0/0
2	SAH	C	403	-	-	0/7/31/31	0/3/3/3
3	SNY	C	603	-	-	0/8/8/8	0/1/1/1
2	SAH	D	404	-	-	0/7/31/31	0/3/3/3
4	BME	D	4089	1	-	0/1/1/1	0/0/0/0
4	BME	D	4295	1	-	0/1/1/1	0/0/0/0
3	SNY	D	604	-	-	0/8/8/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	SAH	C8-N7	-2.31	1.30	1.34
2	C	403	SAH	C8-N7	-2.19	1.30	1.34
2	A	401	SAH	C8-N7	-2.04	1.30	1.34
3	D	604	SNY	C2-C1	2.04	1.43	1.39
2	C	403	SAH	O4'-C1'	2.16	1.43	1.41
3	B	602	SNY	C2-C3	2.26	1.43	1.38
3	B	602	SNY	C2-C1	2.33	1.43	1.39
3	A	601	SNY	C2-C1	2.47	1.44	1.39
3	C	603	SNY	C2-C1	2.53	1.44	1.39
3	A	601	SNY	C2-C3	2.55	1.43	1.38
3	D	604	SNY	C2-C3	2.55	1.43	1.38
3	C	603	SNY	C2-C3	2.59	1.43	1.38
2	A	401	SAH	O4'-C1'	2.97	1.45	1.41
2	D	404	SAH	O4'-C1'	3.06	1.45	1.41
2	B	402	SAH	O4'-C1'	3.31	1.45	1.41
3	B	602	SNY	C5-C4	7.20	1.50	1.40
3	A	601	SNY	C5-C4	7.33	1.50	1.40
3	D	604	SNY	C3-C4	7.43	1.50	1.40
3	C	603	SNY	C3-C4	7.47	1.50	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	SNY	C5-C4	7.51	1.50	1.40
3	D	604	SNY	C5-C4	7.67	1.50	1.40
3	A	601	SNY	C3-C4	8.00	1.51	1.40
3	B	602	SNY	C3-C4	8.00	1.51	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	N3-C2-N1	-10.02	121.22	128.89
2	B	402	SAH	N3-C2-N1	-10.01	121.23	128.89
2	C	403	SAH	N3-C2-N1	-9.92	121.30	128.89
2	D	404	SAH	N3-C2-N1	-9.81	121.38	128.89
2	B	402	SAH	C4'-O4'-C1'	-3.37	106.02	109.72
2	A	401	SAH	C4'-O4'-C1'	-3.16	106.24	109.72
2	D	404	SAH	C4'-O4'-C1'	-3.14	106.27	109.72
2	C	403	SAH	C4'-O4'-C1'	-3.04	106.38	109.72
3	C	603	SNY	O9-C9-C8	-2.67	118.67	125.51
3	D	604	SNY	O9-C9-C8	-2.59	118.88	125.51
3	B	602	SNY	O9-C9-C8	-2.54	119.02	125.51
3	A	601	SNY	O5-C5-C6	-2.50	119.95	124.21
3	C	603	SNY	O5-C5-C6	-2.49	119.97	124.21
2	C	403	SAH	C4-C5-N7	-2.45	107.22	109.48
3	D	604	SNY	O5-C5-C6	-2.43	120.06	124.21
2	A	401	SAH	C4-C5-N7	-2.42	107.26	109.48
3	A	601	SNY	O9-C9-C8	-2.40	119.36	125.51
3	B	602	SNY	O5-C5-C6	-2.36	120.17	124.21
2	B	402	SAH	C4-C5-N7	-2.19	107.46	109.48
2	D	404	SAH	C4-C5-N7	-2.16	107.49	109.48
2	B	402	SAH	CB-CG-SD	-2.12	109.48	113.57
2	A	401	SAH	CB-CG-SD	-2.05	109.62	113.57
3	B	602	SNY	C5M-O5-C5	2.02	120.60	117.54
2	B	402	SAH	O4'-C1'-N9	2.13	112.55	108.10
3	D	604	SNY	C5M-O5-C5	2.16	120.82	117.54
2	A	401	SAH	O4'-C1'-N9	2.54	113.42	108.10
3	B	602	SNY	C3M-O3-C3	3.02	122.13	117.54
3	A	601	SNY	C3M-O3-C3	3.50	122.85	117.54
3	C	603	SNY	C3M-O3-C3	3.53	122.90	117.54
3	D	604	SNY	C3M-O3-C3	3.67	123.10	117.54
3	D	604	SNY	O3-C3-C4	4.29	118.79	114.47
3	C	603	SNY	O3-C3-C4	4.38	118.88	114.47
3	A	601	SNY	O3-C3-C4	4.63	119.13	114.47
3	B	602	SNY	O3-C3-C4	5.23	119.73	114.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	SNY	O5-C5-C4	5.89	120.40	114.47
3	C	603	SNY	O5-C5-C4	6.04	120.55	114.47
3	A	601	SNY	O5-C5-C4	6.07	120.58	114.47
3	D	604	SNY	O5-C5-C4	6.15	120.66	114.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1089	BME	2	0
4	A	1295	BME	1	0
3	A	601	SNY	1	0
4	B	2089	BME	1	0
4	B	2295	BME	4	0
3	B	602	SNY	1	0
4	C	3089	BME	1	0
3	C	603	SNY	1	0
4	D	4295	BME	1	0
3	D	604	SNY	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	357/364 (98%)	-0.12	7 (1%) 68 67	15, 25, 49, 72	0
1	B	356/364 (97%)	0.01	12 (3%) 49 46	17, 27, 53, 96	0
1	C	357/364 (98%)	-0.16	7 (1%) 68 67	14, 23, 46, 71	0
1	D	351/364 (96%)	-0.20	6 (1%) 73 72	15, 25, 46, 81	0
All	All	1421/1456 (97%)	-0.12	32 (2%) 64 62	14, 25, 49, 96	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	ALA	6.0
1	D	10	ALA	5.2
1	B	306	SER	4.9
1	B	9	ALA	4.4
1	C	9	ALA	4.3
1	B	303	ALA	4.3
1	C	6	ALA	3.9
1	B	7	ASP	3.8
1	A	5	ALA	3.6
1	A	4	THR	3.4
1	B	305	PRO	3.3
1	A	50	GLY	3.3
1	B	6	ALA	3.0
1	D	302	GLU	3.0
1	A	7	ASP	3.0
1	A	9	ALA	2.7
1	D	303	ALA	2.7
1	B	10	ALA	2.7
1	B	302	GLU	2.6
1	A	10	ALA	2.5
1	D	193	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	11	SER	2.3
1	C	66	ALA	2.3
1	B	8	MET	2.3
1	B	51	LYS	2.3
1	C	10	ALA	2.3
1	D	63	PRO	2.2
1	B	300	ASN	2.2
1	C	197	GLY	2.2
1	A	6	ALA	2.1
1	C	4	THR	2.1
1	B	198	LEU	2.1

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 carbohydrates 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. 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	BME	D	4295	4/4	0.94	0.31	26.39	8,10,12,16	4
4	BME	A	1295	4/4	0.83	0.33	24.31	10,12,13,17	4
4	BME	C	3089	4/4	0.82	0.49	23.33	16,22,23,24	4
4	BME	B	2295	4/4	0.82	0.47	22.16	29,29,30,31	4
4	BME	C	3295	4/4	0.90	0.32	20.58	9,9,10,17	4
4	BME	B	2089	4/4	0.94	0.30	9.81	10,10,11,11	4
4	BME	A	1089	4/4	0.80	0.56	6.20	29,29,32,33	4
4	BME	D	4089	4/4	0.94	0.24	4.21	2,2,5,10	4
3	SNY	B	602	15/15	0.95	0.10	0.50	16,23,29,29	0
2	SAH	C	403	26/26	0.97	0.08	0.14	13,19,24,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SAH	B	402	26/26	0.95	0.09	-0.03	21,24,31,37	0
3	SNY	C	603	15/15	0.96	0.09	-0.38	15,17,19,21	0
2	SAH	D	404	26/26	0.96	0.07	-0.63	15,20,27,31	0
2	SAH	A	401	26/26	0.97	0.07	-0.75	15,21,26,30	0
3	SNY	A	601	15/15	0.97	0.07	-0.85	14,17,21,23	0
3	SNY	D	604	15/15	0.95	0.08	-0.88	12,19,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.