



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:21 AM GMT

PDB ID : 3AEJ
Title : Reaction intermediate structure of *Entamoeba histolytica* methionine gamma-lyase 1 tetramer containing Michaelis complex and methionine-pyridoxal-5'-phosphate
Authors : Karaki, T.; Sato, D.; Shimizu, A.; Nozaki, T.; Harada, S.
Deposited on : 2010-02-10
Resolution : 2.59 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

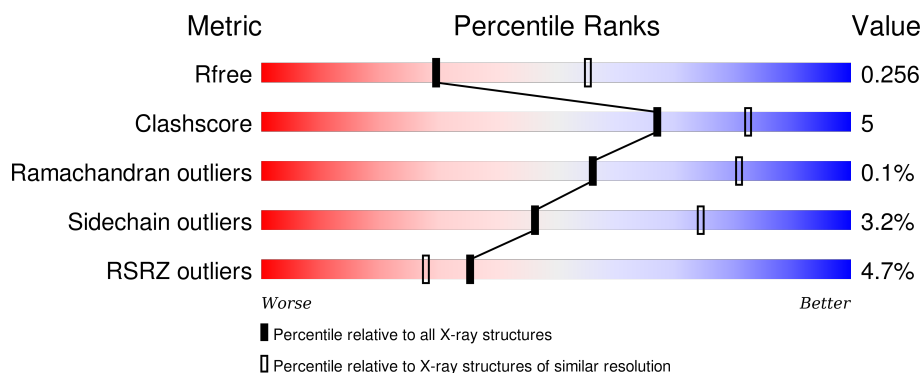
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	389	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>
1	B	389	<div> <div>5%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>
1	D	389	<div> <div>8%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
2	C	389	<div> <div>3%</div> <div>85%</div> <div>14%</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
3	AA5	B	2002	-	-	-	X
3	AA5	D	2004	-	-	-	X
6	MET	C	2003	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12308 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 Methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	1	0
			2952	1878	497	553	24			
1	B	386	Total	C	N	O	S	0	1	0
			2937	1867	495	551	24			
1	D	384	Total	C	N	O	S	0	0	0
			2920	1857	492	548	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	LEU	SER	SEE REMARK 999	UNP Q86D28
B	808	LEU	SER	SEE REMARK 999	UNP Q86D28
D	1808	LEU	SER	SEE REMARK 999	UNP Q86D28

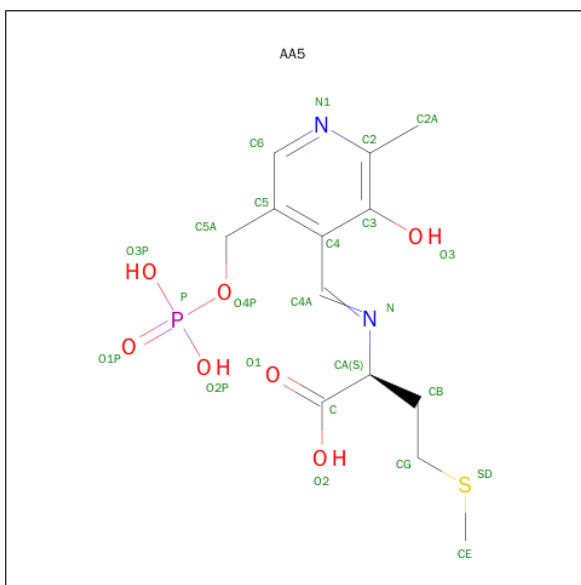
- Molecule 2 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	387	Total	C	N	O	P S	0	1	0
			2967	1886	498	558	1 24			

There is a discrepancy between the modelled and reference sequences:

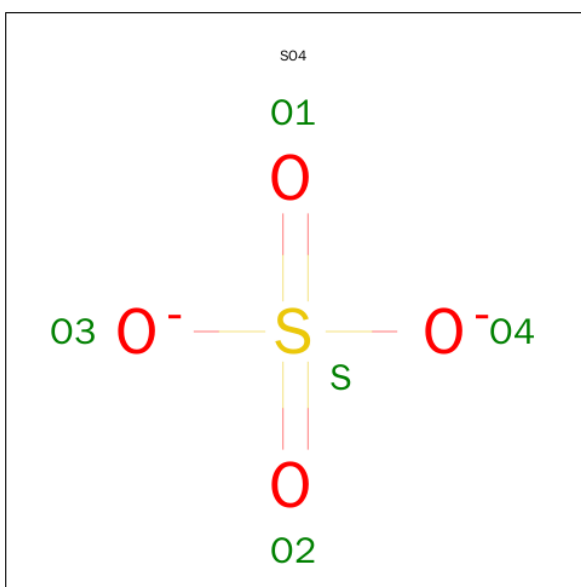
Chain	Residue	Modelled	Actual	Comment	Reference
C	1308	LEU	SER	SEE REMARK 999	UNP Q86D28

- Molecule 3 is N-[(3-HYDROXY-2-METHYL-5-{[(TRIHIDROXYPHOSPHORANYL)OXY]METHYL}PYRIDIN-4-YL)METHYLENE]METHIONINE (three-letter code: AA5) (formula: C₁₃H₁₉N₂O₇PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 24	C 13	N 2	O 7	P 1	S 1	0	0
3	B	1	Total 24	C 13	N 2	O 7	P 1	S 1	0	0
3	D	1	Total 24	C 13	N 2	O 7	P 1	S 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



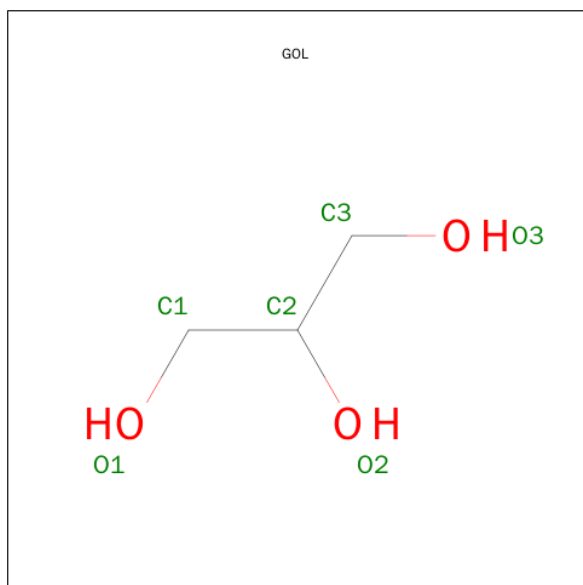
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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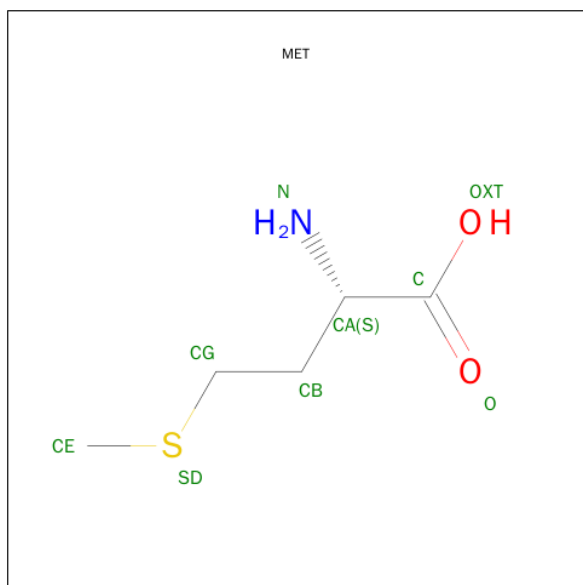
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

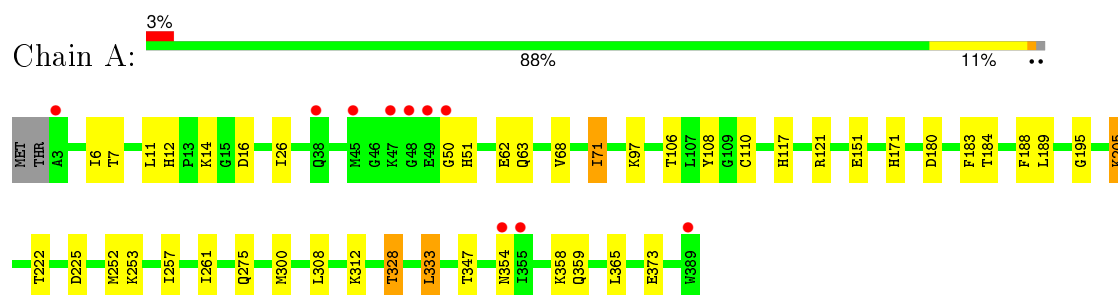
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total	O	0	0
			123	123		
7	B	78	Total	O	0	0
			78	78		
7	C	134	Total	O	0	0
			134	134		
7	D	84	Total	O	0	0
			84	84		

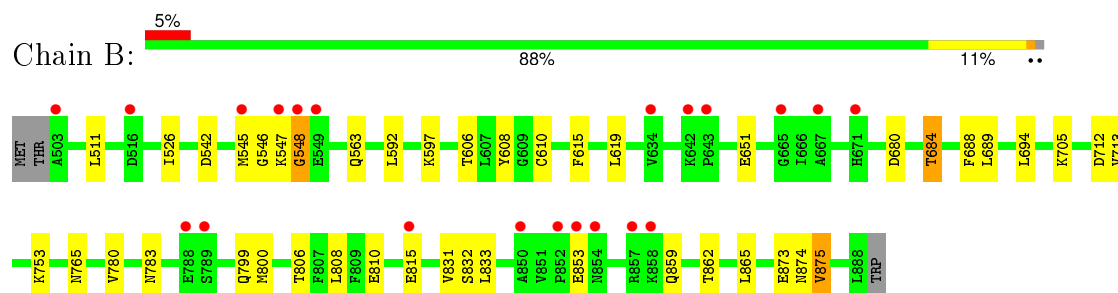
3 Residue-property plots

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.

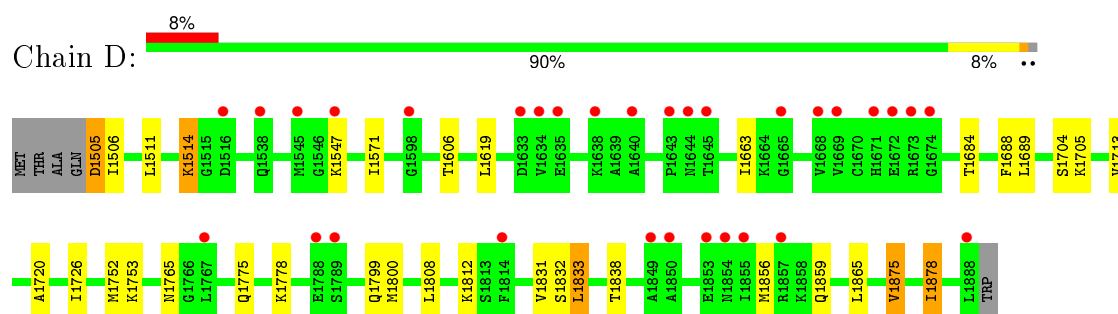
• Molecule 1: Methionine gamma-lyase



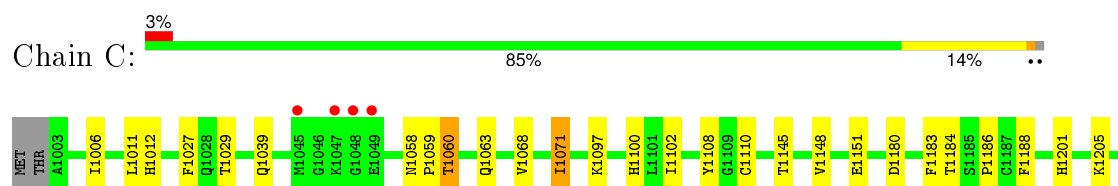
• Molecule 1: Methionine gamma-lyase

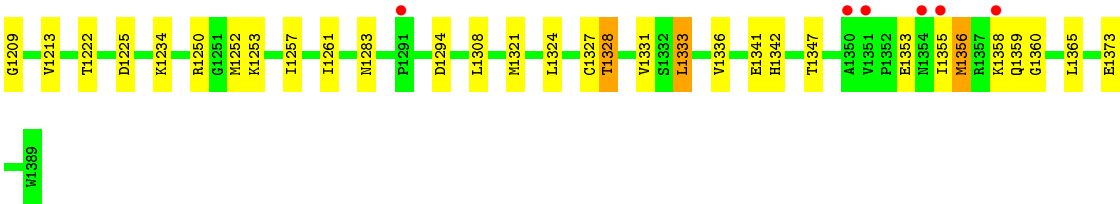


• Molecule 1: Methionine gamma-lyase



• Molecule 2: Methionine gamma-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.74Å 85.36Å 113.66Å 90.00° 101.92° 90.00°	Depositor
Resolution (Å)	39.04 – 2.59 39.04 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.04-2.59) 99.4 (39.04-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.209 , 0.256 0.208 , 0.256	Depositor DCC
R_{free} test set	2921 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57685 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12308	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.55% 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, 0.375 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: AA5, GOL, LLP, SO4

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	0.32	0/3018	0.48	0/4080
1	B	0.32	0/3001	0.46	0/4057
1	D	0.32	0/2981	0.46	0/4030
2	C	0.32	0/3008	0.48	0/4066
All	All	0.32	0/12008	0.47	0/16233

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	2952	0	2957	32	0
1	B	2937	0	2947	30	0
1	D	2920	0	2929	22	0
2	C	2967	0	2962	41	0
3	A	24	0	16	4	0
3	B	24	0	15	2	0
3	D	24	0	15	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	6	0	8	1	0
5	C	6	0	8	0	0
6	C	9	0	8	3	0
7	A	123	0	0	3	0
7	B	78	0	0	1	0
7	C	134	0	0	3	0
7	D	84	0	0	0	0
All	All	12308	0	11865	114	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 5.

All (114) 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)
2:C:1353:GLU:HA	2:C:1356:MET:HB3	1.66	0.78
2:C:1071:ILE:HD11	2:C:1252:MET:HE1	1.69	0.74
1:D:1808:LEU:HD21	1:D:1865:LEU:HD13	1.69	0.73
2:C:1347:THR:HG22	6:C:2003:MET:HB3	1.70	0.73
1:B:874:ASN:HB2	1:D:1505:ASP:HB2	1.72	0.70
1:A:261:ILE:HD11	2:C:1257:ILE:HG12	1.72	0.70
1:A:71:ILE:HD11	1:A:252:MET:CE	2.22	0.69
1:B:651:GLU:HG2	1:B:680:ASP:HB3	1.72	0.69
2:C:1071:ILE:HD11	2:C:1252:MET:CE	2.24	0.68
2:C:1308:LEU:HD21	2:C:1365:LEU:HD13	1.74	0.68
1:D:1705:LYS:HZ2	3:D:2004:AA5:HA	1.58	0.68
1:A:205:LYS:HZ1	3:A:2001:AA5:HA	1.62	0.64
1:B:545:MET:H	1:B:546:GLY:HA2	1.62	0.64
1:D:1808:LEU:HD11	1:D:1865:LEU:HB3	1.80	0.63
1:A:11:LEU:HD12	2:C:1373:GLU:HG3	1.79	0.62
1:B:610:CYS:SG	2:C:1234:LYS:NZ	2.71	0.62
1:D:1511:LEU:HD23	1:D:1753:LYS:HD2	1.80	0.62
1:D:1606:THR:HA	1:D:1859:GLN:HE21	1.65	0.61
1:D:1506:ILE:HG21	1:D:1571:ILE:HD13	1.82	0.60
1:A:222:THR:HG22	1:A:225:ASP:H	1.66	0.60
1:A:71:ILE:HD11	1:A:252:MET:HE1	1.82	0.60
1:B:705:LYS:HZ1	3:B:2002:AA5:HA	1.66	0.60
1:D:1705:LYS:HE3	3:D:2004:AA5:H4A	1.83	0.59
1:A:205:LYS:HG2	1:A:333:LEU:HG	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:GLU:HG3	1:D:1511:LEU:HD12	1.85	0.59
1:A:257:ILE:HG12	2:C:1261:ILE:HD11	1.85	0.59
1:A:308:LEU:HD21	1:A:365:LEU:HD13	1.84	0.58
1:A:51:HIS:HE1	1:A:62:GLU:OE1	1.88	0.57
1:A:328:THR:HG22	7:A:3014:HOH:O	2.05	0.56
1:D:1684:THR:HG22	1:D:1688:PHE:HB2	1.86	0.56
2:C:1068:VAL:HA	2:C:1071:ILE:HD11	1.86	0.56
1:A:373:GLU:HG3	2:C:1011:LEU:HD12	1.86	0.56
2:C:1222:THR:HG22	2:C:1225:ASP:H	1.70	0.56
1:B:808:LEU:HD11	1:B:865:LEU:HB3	1.87	0.56
1:A:184:THR:HG22	1:A:188:PHE:HB2	1.87	0.55
2:C:1328:THR:HG22	7:C:3001:HOH:O	2.06	0.55
1:B:608:TYR:CE1	3:B:2002:AA5:HB1	2.41	0.55
2:C:1184:THR:HG22	2:C:1188:PHE:HB2	1.89	0.54
1:A:71:ILE:HD11	1:A:252:MET:HE2	1.90	0.54
1:B:545:MET:N	1:B:546:GLY:HA2	2.18	0.54
2:C:1308:LEU:HD11	2:C:1365:LEU:HB3	1.90	0.54
1:A:11:LEU:HD22	2:C:1336:VAL:HG12	1.90	0.53
1:B:808:LEU:HD21	1:B:865:LEU:HD13	1.91	0.53
1:D:1514:LYS:HD3	1:D:1514:LYS:H	1.75	0.52
1:A:151:GLU:HG2	1:A:180:ASP:HB3	1.92	0.52
1:D:1838:THR:HG21	1:D:1878:ILE:HD13	1.92	0.51
1:A:205:LYS:NZ	3:A:2001:AA5:HA	2.26	0.51
1:B:542:ASP:HB3	1:B:547:LYS:O	2.11	0.51
2:C:1027:PHE:H	2:C:1060:THR:HG21	1.76	0.50
1:B:592:LEU:HD21	1:B:619:LEU:HD22	1.92	0.50
1:B:705:LYS:HD2	1:B:833:LEU:HG	1.93	0.50
1:B:511:LEU:HD23	1:B:753:LYS:HG3	1.93	0.50
1:A:205:LYS:NZ	3:A:2001:AA5:H4A	2.27	0.50
1:B:597:LYS:HE3	2:C:1097:LYS:HE3	1.94	0.50
7:B:3010:HOH:O	2:C:1331:VAL:HG22	2.11	0.50
1:B:606:THR:HA	1:B:859:GLN:HE21	1.76	0.50
2:C:1068:VAL:HA	2:C:1071:ILE:CD1	2.42	0.49
2:C:1359:GLN:N	2:C:1360:GLY:HA2	2.26	0.49
1:D:1704:SER:HB2	1:D:1705:LYS:HE2	1.94	0.49
2:C:1027:PHE:H	2:C:1060:THR:CG2	2.25	0.49
2:C:1250:ARG:O	2:C:1253:LYS:HB2	2.13	0.49
1:B:862:THR:H	1:B:865:LEU:HD12	1.79	0.48
2:C:1108:TYR:HE1	6:C:2003:MET:HB2	1.78	0.48
1:A:6:ILE:HG12	1:A:71:ILE:HG23	1.95	0.48
1:B:542:ASP:O	1:B:546:GLY:HA2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HA	1:A:71:ILE:CD1	2.45	0.47
1:A:171:HIS:CE1	1:A:195:GLY:O	2.68	0.47
1:A:108:TYR:CE2	1:A:110:CYS:HB2	2.50	0.47
1:D:1663:ILE:H	1:D:1799:GLN:HE22	1.61	0.47
2:C:1102:ILE:O	2:C:1148:VAL:HA	2.14	0.46
2:C:1108:TYR:CE2	2:C:1110:CYS:HB2	2.50	0.46
1:D:1689:LEU:HD13	1:D:1800:MET:HG2	1.96	0.46
1:B:608:TYR:CE2	1:B:610:CYS:HB2	2.50	0.46
1:A:12:HIS:HE1	7:C:3001:HOH:O	1.99	0.46
1:A:7:THR:O	1:A:11:LEU:HG	2.16	0.45
1:D:1778:LYS:HA	1:D:1812:LYS:HE3	1.97	0.45
2:C:1006:ILE:HG12	2:C:1071:ILE:HG23	1.98	0.45
1:D:1720:ALA:HB3	1:D:1726:ILE:HB	1.98	0.45
1:D:1705:LYS:HD2	1:D:1833:LEU:HG	1.97	0.45
7:A:3014:HOH:O	2:C:1012:HIS:HE1	2.00	0.45
2:C:1321:MET:CE	2:C:1342:HIS:HB2	2.46	0.45
2:C:1100:HIS:HB3	2:C:1145:THR:HA	1.99	0.45
1:A:106:THR:HG22	1:A:359:GLN:HG2	1.99	0.45
2:C:1151:GLU:HG2	2:C:1180:ASP:HB3	1.99	0.44
1:B:689:LEU:HD13	1:B:800:MET:HG2	1.99	0.44
2:C:1186:PRO:HD3	2:C:1201:HIS:CE1	2.52	0.44
1:A:68:VAL:HA	1:A:71:ILE:HD11	2.00	0.44
2:C:1108:TYR:CE1	6:C:2003:MET:HB2	2.52	0.44
2:C:1205:LLP:HD3	2:C:1333:LEU:HG	1.98	0.44
1:A:347:THR:HG22	3:A:2001:AA5:HG2	2.00	0.43
1:B:684:THR:HG22	1:B:688:PHE:HB2	1.99	0.43
1:D:1514:LYS:CD	1:D:1514:LYS:H	2.31	0.43
1:A:26:ILE:HB	1:B:526:ILE:HB	1.98	0.43
2:C:1331:VAL:HG12	2:C:1341:GLU:HG3	2.00	0.43
1:B:712:ASP:HA	2:C:1029:THR:HA	2.00	0.43
2:C:1058:ASN:HA	2:C:1059:PRO:HD3	1.94	0.43
2:C:1222:THR:HG21	7:C:3403:HOH:O	2.18	0.43
2:C:1209:GLY:O	2:C:1336:VAL:HG23	2.20	0.42
1:A:253:LYS:HE3	7:A:3083:HOH:O	2.18	0.42
1:A:189:LEU:HD13	1:A:300:MET:HG2	2.01	0.42
1:B:694:LEU:HD13	1:B:799:GLN:HE21	1.84	0.42
1:D:1765:ASN:ND2	1:D:1875:VAL:HG22	2.35	0.42
1:B:765:ASN:ND2	1:B:875:VAL:HG22	2.35	0.41
1:B:806:THR:HG21	1:B:833:LEU:HD22	2.02	0.41
1:A:312:LYS:HD3	5:A:2009:GOL:H31	2.02	0.41
1:A:117:HIS:O	1:A:121:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:PHE:HA	1:B:619:LEU:HG	2.02	0.41
2:C:1324:LEU:HD13	2:C:1327:CYS:HB2	2.03	0.41
1:B:831:VAL:O	1:B:832:SER:HB3	2.19	0.41
1:B:547:LYS:HA	1:B:548:GLY:HA2	1.74	0.40
1:D:1831:VAL:O	1:D:1832:SER:HB3	2.22	0.40
1:D:1506:ILE:CG2	1:D:1571:ILE:HD13	2.51	0.40
1:B:780:VAL:HB	1:B:810:GLU:HB3	2.04	0.40
2:C:1355:ILE:HA	2:C:1358:LYS:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/389 (99%)	376 (97%)	9 (2%)	1 (0%)	46	72
1	B	385/389 (99%)	376 (98%)	8 (2%)	1 (0%)	46	72
1	D	382/389 (98%)	371 (97%)	11 (3%)	0	100	100
2	C	385/389 (99%)	377 (98%)	8 (2%)	0	100	100
All	All	1538/1556 (99%)	1500 (98%)	36 (2%)	2 (0%)	56	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	GLY
1	B	548	GLY

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/322 (100%)	309 (96%)	12 (4%)	41	69
1	B	320/322 (99%)	313 (98%)	7 (2%)	60	83
1	D	318/322 (99%)	307 (96%)	11 (4%)	43	71
2	C	320/321 (100%)	309 (97%)	11 (3%)	44	72
All	All	1279/1287 (99%)	1238 (97%)	41 (3%)	46	74

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	16	ASP
1	A	63	GLN
1	A	71	ILE
1	A	97	LYS
1	A	183	PHE
1	A	205	LYS
1	A	275	GLN
1	A	328	THR
1	A	333	LEU
1	A	354	ASN
1	A	358	LYS
1	B	563	GLN
1	B	684	THR
1	B	713	VAL
1	B	783	ASN
1	B	815	GLU
1	B	853	GLU
1	B	875	VAL
2	C	1039	GLN
2	C	1060	THR
2	C	1063	GLN
2	C	1071	ILE
2	C	1183	PHE
2	C	1213	VAL
2	C	1283	ASN
2	C	1294	ASP
2	C	1328	THR

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Mol	Chain	Res	Type
2	C	1333	LEU
2	C	1356	MET
1	D	1505	ASP
1	D	1514	LYS
1	D	1547	LYS
1	D	1619	LEU
1	D	1713	VAL
1	D	1752	MET
1	D	1775	GLN
1	D	1833	LEU
1	D	1856	MET
1	D	1875	VAL
1	D	1878	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	100	HIS
1	A	171	HIS
1	A	265	ASN
1	A	275	GLN
1	A	293	HIS
1	A	299	GLN
1	A	354	ASN
1	A	374	ASN
1	B	504	GLN
1	B	600	HIS
1	B	760	GLN
1	B	765	ASN
1	B	783	ASN
1	B	793	HIS
1	B	799	GLN
1	B	842	HIS
1	B	874	ASN
2	C	1039	GLN
2	C	1063	GLN
2	C	1100	HIS
2	C	1265	ASN
2	C	1283	ASN
2	C	1293	HIS
2	C	1299	GLN

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Mol	Chain	Res	Type
2	C	1323	HIS
2	C	1348	HIS
2	C	1359	GLN
2	C	1374	ASN
1	D	1600	HIS
1	D	1765	ASN
1	D	1793	HIS
1	D	1799	GLN
1	D	1854	ASN
1	D	1859	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LLP	C	1205	2	23,24,25	1.74	5 (21%)	28,32,34	1.87	5 (17%)

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	LLP	C	1205	2	-	0/15/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1205	LLP	O3-C3	-5.71	1.23	1.37
2	C	1205	LLP	C6-N1	2.14	1.39	1.34
2	C	1205	LLP	C4'-NZ	2.15	1.34	1.27
2	C	1205	LLP	C2-N1	2.28	1.38	1.34
2	C	1205	LLP	C4-C4'	2.49	1.51	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1205	LLP	C4-C4'-NZ	-2.76	109.72	125.06
2	C	1205	LLP	CE-NZ-C4'	-2.49	111.77	118.97
2	C	1205	LLP	O-C-CA	-2.28	119.55	125.49
2	C	1205	LLP	C5-C6-N1	-2.14	120.14	123.86
2	C	1205	LLP	OP4-C5'-C5	7.40	121.22	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1205	LLP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	AA5	A	2001	-	20,24,24	3.14	2 (10%)	22,33,33	1.23	3 (13%)
4	SO4	A	2005	-	4,4,4	0.23	0	6,6,6	0.09	0
5	GOL	A	2009	-	5,5,5	0.33	0	5,5,5	0.38	0
3	AA5	B	2002	-	20,24,24	3.25	2 (10%)	22,33,33	1.00	0
4	SO4	B	2006	-	4,4,4	0.24	0	6,6,6	0.07	0
6	MET	C	2003	-	5,8,8	0.17	0	3,9,9	0.29	0
4	SO4	C	2007	-	4,4,4	0.21	0	6,6,6	0.08	0
5	GOL	C	2010	-	5,5,5	0.33	0	5,5,5	0.21	0
3	AA5	D	2004	-	20,24,24	3.13	2 (10%)	22,33,33	1.10	1 (4%)
4	SO4	D	2008	-	4,4,4	0.22	0	6,6,6	0.09	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	AA5	A	2001	-	-	0/15/19/19	0/1/1/1
4	SO4	A	2005	-	-	0/0/0/0	0/0/0/0
5	GOL	A	2009	-	-	0/4/4/4	0/0/0/0
3	AA5	B	2002	-	-	0/15/19/19	0/1/1/1
4	SO4	B	2006	-	-	0/0/0/0	0/0/0/0
6	MET	C	2003	-	-	0/4/8/8	0/0/0/0
4	SO4	C	2007	-	-	0/0/0/0	0/0/0/0
5	GOL	C	2010	-	-	0/4/4/4	0/0/0/0
3	AA5	D	2004	-	-	0/15/19/19	0/1/1/1
4	SO4	D	2008	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	AA5	C4-C3	6.47	1.48	1.40
3	D	2004	AA5	C4-C3	6.48	1.48	1.40
3	B	2002	AA5	C4-C3	7.03	1.49	1.40
3	D	2004	AA5	C3-C2	11.95	1.49	1.40
3	A	2001	AA5	C3-C2	12.05	1.49	1.40
3	B	2002	AA5	C3-C2	12.33	1.49	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	AA5	C3-C4-C4A	-2.16	117.36	120.16
3	D	2004	AA5	O3-C3-C2	2.15	121.40	117.66
3	A	2001	AA5	C5-C4-C4A	2.16	124.63	121.52
3	A	2001	AA5	O3-C3-C2	2.29	121.64	117.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	AA5	4	0
5	A	2009	GOL	1	0
3	B	2002	AA5	2	0
6	C	2003	MET	3	0
3	D	2004	AA5	2	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	387/389 (99%)	0.06	10 (2%) 59 53	14, 20, 43, 62	1 (0%)
1	B	386/389 (99%)	0.31	21 (5%) 29 22	18, 31, 53, 66	1 (0%)
1	D	384/389 (98%)	0.38	31 (8%) 15 10	18, 32, 56, 66	0
2	C	386/389 (99%)	0.06	10 (2%) 59 53	14, 20, 41, 57	1 (0%)
All	All	1543/1556 (99%)	0.20	72 (4%) 35 28	14, 25, 51, 66	3 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1634	VAL	3.8
1	A	47	LYS	3.7
1	B	548	GLY	3.6
2	C	1047	LYS	3.5
1	D	1857	ARG	3.5
1	D	1671	HIS	3.4
1	B	853	GLU	3.4
1	B	516	ASP	3.4
1	B	545	MET	3.4
1	B	854	ASN	3.3
1	B	857	ARG	3.3
1	B	850	ALA	3.3
1	D	1854	ASN	3.2
2	C	1045	MET	3.2
1	B	858	LYS	3.2
2	C	1049	GLU	3.1
1	D	1643	PRO	3.1
1	A	49	GLU	3.1
2	C	1351	VAL	3.0
1	A	3	ALA	3.0
2	C	1354	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	788	GLU	2.9
1	B	634	VAL	2.8
1	A	354	ASN	2.8
1	B	503	ALA	2.8
1	D	1547	LYS	2.8
1	A	50	GLY	2.7
1	B	547	LYS	2.7
1	D	1850	ALA	2.7
2	C	1048	GLY	2.7
1	D	1888	LEU	2.6
1	D	1789	SER	2.6
1	B	852	PRO	2.6
1	D	1849	ALA	2.6
1	D	1516	ASP	2.5
1	D	1598	GLY	2.5
1	D	1674	GLY	2.5
1	B	671	HIS	2.5
2	C	1350	ALA	2.5
1	D	1635	GLU	2.5
1	B	665	GLY	2.5
1	A	45	MET	2.5
2	C	1291	PRO	2.4
1	A	38	GLN	2.4
1	D	1665	GLY	2.4
2	C	1355	ILE	2.4
1	D	1788	GLU	2.4
1	D	1855	ILE	2.4
1	D	1644	ASN	2.4
1	D	1814	PHE	2.4
1	D	1673	ARG	2.4
1	D	1538	GLN	2.4
1	D	1645	THR	2.4
1	D	1669	VAL	2.3
1	D	1545	MET	2.3
1	D	1640	ALA	2.3
1	D	1672	GLU	2.3
1	D	1668	VAL	2.3
1	B	667	ALA	2.3
1	D	1638	LYS	2.3
1	D	1633	ASP	2.2
2	C	1358	LYS	2.2
1	D	1853	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	643	PRO	2.2
1	A	355	ILE	2.2
1	B	815	GLU	2.2
1	B	549	GLU	2.1
1	B	789	SER	2.1
1	A	389	TRP	2.1
1	B	642	LYS	2.1
1	A	48	GLY	2.0
1	D	1767	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	LLP	C	1205	24/25	0.96	0.16	-	15,16,17,18	6

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
6	MET	C	2003	9/9	0.80	0.32	6.34	36,36,38,38	0
3	AA5	D	2004	24/24	0.87	0.29	2.81	36,40,41,42	0
3	AA5	B	2002	24/24	0.86	0.27	2.45	32,36,38,40	0
3	AA5	A	2001	24/24	0.91	0.22	1.80	20,25,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	2009	6/6	0.86	0.17	0.68	36,36,37,37	0
5	GOL	C	2010	6/6	0.87	0.16	0.52	46,46,46,46	0
4	SO4	C	2007	5/5	0.91	0.28	-	59,59,60,60	0
4	SO4	D	2008	5/5	0.89	0.33	-	65,65,65,65	0
4	SO4	B	2006	5/5	0.93	0.28	-	68,68,68,68	0
4	SO4	A	2005	5/5	0.94	0.21	-	63,63,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.