Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:19 PM GMT

PDB ID	:	1F4D
Title	:	CRYSTAL STRUCTURE OF E. COLI THYMIDYLATE SYNTHASE C146S, L143C COVALENTLY MODIFIED AT C143 WITH N-[TOSYL-D-PROLINYL]AMINO-ETHANETHIOL
Authors	:	Erlanson, D.A.; Braisted, A.C.; Raphael, D.R.; Randal, M.; Stroud, R.M.; Gordon, E.; Wells, J.A.
Deposited on	:	2000-06-07
Resolution	:	2.15 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

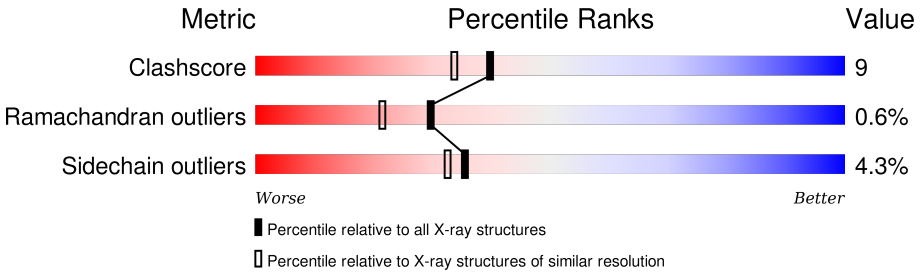
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.15 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))
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	77% 19%
1	B	264	72% 23% 5%

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	GOL	A	501	-	-	X	-
4	GOL	B	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4682 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.

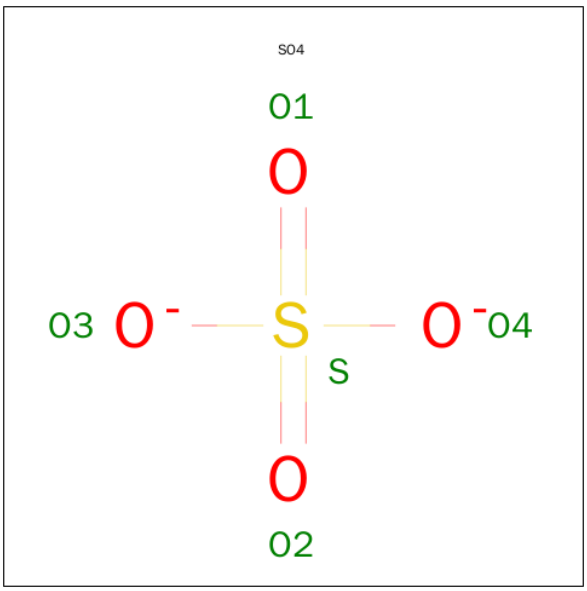
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	1	0
			2156	1375	373	396	12			
1	B	264	Total	C	N	O	S	0	1	0
			2155	1374	372	397	12			

There are 6 discrepancies between the modelled and reference sequences:

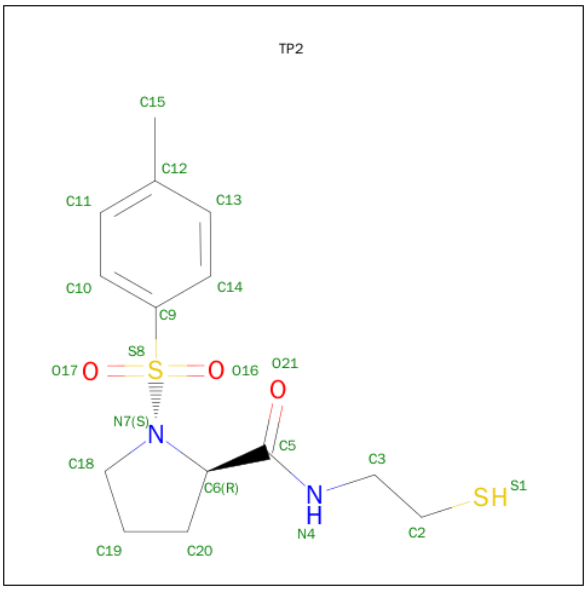
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	ENGINEERED	UNP P0A884
A	143	CYS	LEU	ENGINEERED	UNP P0A884
A	146	SER	CYS	ENGINEERED	UNP P0A884
B	1	CXM	MET	ENGINEERED	UNP P0A884
B	143	CYS	LEU	ENGINEERED	UNP P0A884
B	146	SER	CYS	ENGINEERED	UNP P0A884

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



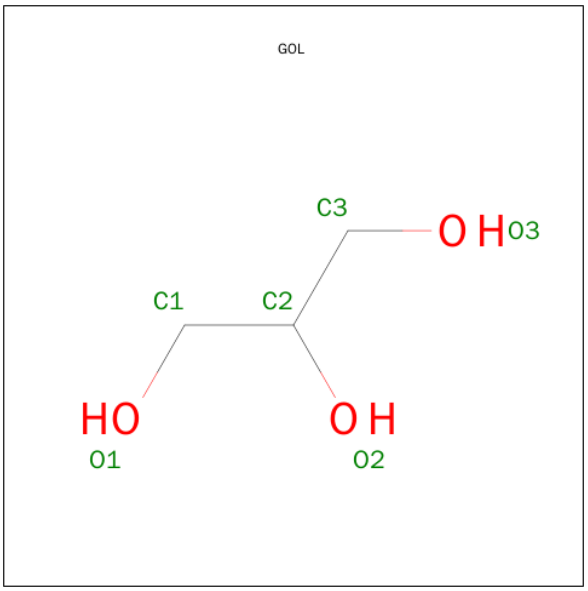
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is N-[TOSYL-D-PROLINYL]AMINO-ETHANETHIOL (three-letter code: TP2) (formula: $C_{14}H_{20}N_2O_3S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 21 14 2 3 2	0	0
3	B	1	Total C N O S 21 14 2 3 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	179	Total O 179 179	0	0
5	B	118	Total O 118 118	0	0

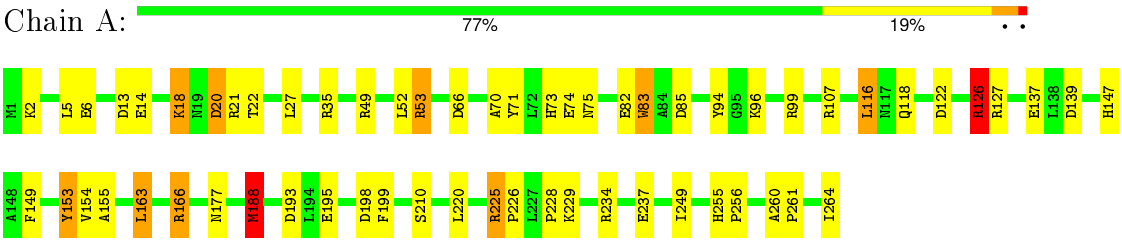
3 Residue-property plots (i)

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

Note EDS was not executed.

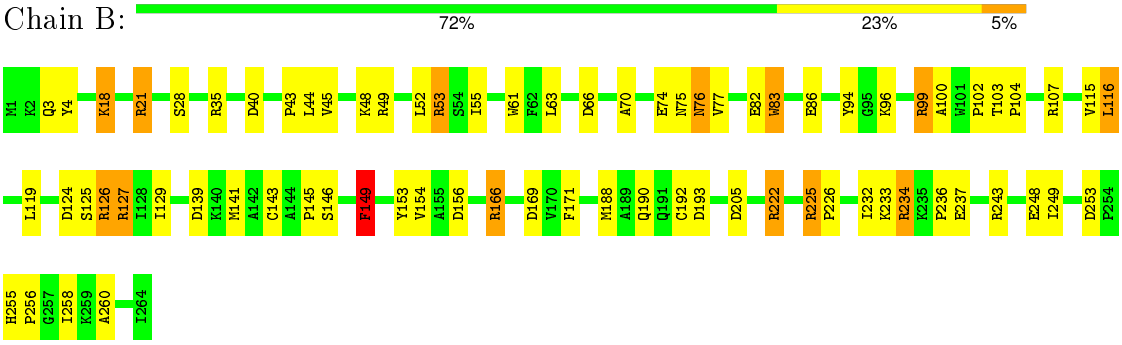
- Molecule 1: THYMIDYLATE SYNTHASE

Chain A:



- Molecule 1: THYMIDYLATE SYNTHASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	126.33Å 126.33Å 67.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.15	Depositor
% Data completeness (in resolution range)	96.7 (10.00-2.15)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4682	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CXM, TP2, 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	0.74	0/2211	1.80	52/3002 (1.7%)
1	B	0.71	1/2209 (0.0%)	1.74	42/2999 (1.4%)
All	All	0.73	1/4420 (0.0%)	1.77	94/6001 (1.6%)

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	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	PHE	CB-CG	-5.20	1.42	1.51

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	ARG	NE-CZ-NH2	-20.50	110.05	120.30
1	B	127	ARG	NE-CZ-NH1	16.18	128.39	120.30
1	B	126	ARG	NE-CZ-NH2	-15.89	112.35	120.30
1	A	127	ARG	NE-CZ-NH2	-14.52	113.04	120.30
1	B	99	ARG	NE-CZ-NH1	-13.72	113.44	120.30
1	A	166	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	A	18	LYS	CA-CB-CG	12.83	141.62	113.40
1	B	107	ARG	CD-NE-CZ	11.89	140.25	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	A	126	ARG	NH1-CZ-NH2	11.22	131.75	119.40
1	B	35	ARG	CD-NE-CZ	11.19	139.26	123.60
1	B	243	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	B	243	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	B	49	ARG	NE-CZ-NH2	10.30	125.45	120.30
1	A	49	ARG	NE-CZ-NH2	9.80	125.20	120.30
1	B	143	CYS	CA-CB-SG	9.68	131.42	114.00
1	A	225	ARG	NE-CZ-NH2	-9.61	115.49	120.30
1	B	222	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	B	166	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	13	ASP	CB-CG-OD2	-9.26	109.96	118.30
1	B	126	ARG	NH1-CZ-NH2	8.82	129.10	119.40
1	B	243	ARG	CD-NE-CZ	8.82	135.95	123.60
1	A	73[A]	HIS	CB-CA-C	8.73	127.86	110.40
1	A	73[B]	HIS	CB-CA-C	8.73	127.86	110.40
1	B	49	ARG	CD-NE-CZ	8.62	135.67	123.60
1	B	53	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	B	169	ASP	CB-CG-OD1	8.36	125.82	118.30
1	A	53	ARG	CD-NE-CZ	8.19	135.07	123.60
1	A	225	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	225	ARG	CD-NE-CZ	7.92	134.69	123.60
1	B	21	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	49	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	A	122	ASP	CB-CG-OD2	7.79	125.31	118.30
1	B	153	TYR	CB-CG-CD2	-7.70	116.38	121.00
1	B	28	SER	N-CA-CB	-7.61	99.09	110.50
1	A	153	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	A	195	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	A	85	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	107	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	B	149	PHE	CA-CB-CG	7.24	131.28	113.90
1	A	83	TRP	CA-CB-CG	-7.19	100.04	113.70
1	B	234	ARG	NE-CZ-NH1	-7.13	116.74	120.30
1	B	49	ARG	NH1-CZ-NH2	-7.02	111.68	119.40
1	B	143	CYS	N-CA-CB	6.99	123.18	110.60
1	B	127	ARG	NH1-CZ-NH2	-6.98	111.72	119.40
1	A	21	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	99	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	166	ARG	NH1-CZ-NH2	6.56	126.61	119.40
1	A	234	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	86	GLU	OE1-CD-OE2	-6.49	115.51	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73[A]	HIS	CB-CG-ND1	-6.49	106.98	123.20
1	A	73[B]	HIS	CB-CG-ND1	-6.49	106.98	123.20
1	A	71	TYR	CB-CG-CD1	-6.47	117.12	121.00
1	A	199	PHE	CB-CG-CD2	-6.37	116.34	120.80
1	A	139	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	66	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	B	139	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	45	VAL	CA-CB-CG1	6.15	120.12	110.90
1	A	13	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	137	GLU	OE1-CD-OE2	-6.14	115.94	123.30
1	A	149	PHE	N-CA-CB	-5.98	99.83	110.60
1	A	107	ARG	NH1-CZ-NH2	-5.96	112.85	119.40
1	A	155	ALA	N-CA-CB	5.92	118.39	110.10
1	A	225	ARG	CG-CD-NE	5.92	124.22	111.80
1	A	163	LEU	CA-CB-CG	5.87	128.79	115.30
1	B	153	TYR	CB-CG-CD1	5.83	124.50	121.00
1	B	205	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	99	ARG	NH1-CZ-NH2	5.77	125.75	119.40
1	A	18	LYS	CB-CA-C	5.77	121.94	110.40
1	B	156	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	193	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	107	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	B	149	PHE	CG-CD1-CE1	5.70	127.07	120.80
1	B	149	PHE	CD1-CG-CD2	-5.69	110.90	118.30
1	A	153	TYR	CB-CG-CD1	5.63	124.38	121.00
1	A	53	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	B	192	CYS	CA-CB-SG	-5.41	104.26	114.00
1	A	147	HIS	CB-CA-C	5.38	121.16	110.40
1	B	76	ASN	CB-CG-OD1	-5.34	110.92	121.60
1	A	53	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	B	234	ARG	CD-NE-CZ	5.31	131.03	123.60
1	B	83	TRP	CA-CB-CG	-5.17	103.87	113.70
1	B	66	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	193	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	B	49	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	71	TYR	CB-CG-CD2	5.13	124.08	121.00
1	A	73[A]	HIS	CB-CG-CD2	5.12	146.69	130.80
1	A	73[B]	HIS	CB-CG-CD2	5.12	146.69	130.80
1	A	188	MET	CA-CB-CG	-5.12	104.59	113.30
1	B	225	ARG	CG-CD-NE	5.08	122.47	111.80
1	A	234	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	4	TYR	CB-CG-CD1	5.02	124.01	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	ASN	CB-CG-OD1	-5.01	111.57	121.60
1	A	21	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLN	Mainchain
1	A	210	SER	Mainchain
1	B	40	ASP	Mainchain
1	B	61	TRP	Mainchain

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	2156	0	2076	39	0
1	B	2155	0	2077	46	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	21	0	19	3	0
3	B	21	0	19	1	0
4	A	6	0	8	4	0
4	B	6	0	8	5	0
5	A	179	0	0	4	0
5	B	118	0	0	5	0
All	All	4682	0	4207	76	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 9.

All (76) 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:3[A]:GLN:OE1	5:B:627:HOH:O	1.61	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HH12	4:A:501:GOL:H11	1.49	0.77
1:B:233:LYS:HD2	1:B:248:GLU:HG2	1.69	0.74
1:B:103:THR:HB	1:B:104:PRO:HD2	1.70	0.73
5:A:678:HOH:O	1:B:18:LYS:HE3	1.90	0.71
1:A:22:THR:HA	5:A:663:HOH:O	1.89	0.71
1:A:70:ALA:O	1:A:74:GLU:HG3	1.91	0.69
1:A:126:ARG:HD3	4:B:502:GOL:H12	1.75	0.68
1:A:166:ARG:NH1	4:A:501:GOL:H11	2.10	0.66
1:B:127:ARG:HD3	5:B:571:HOH:O	1.96	0.65
1:A:126:ARG:HD3	4:B:502:GOL:C1	2.27	0.64
1:B:225:ARG:HD2	1:B:253:ASP:O	1.97	0.64
1:B:116:LEU:HD13	1:B:188:MET:SD	2.38	0.64
1:A:18:LYS:HE2	1:B:124:ASP:OD1	1.99	0.63
1:A:18:LYS:HE3	1:B:154:VAL:O	1.99	0.62
1:B:52:LEU:HD22	1:B:249:ILE:HG21	1.80	0.62
1:B:141:MET:SD	1:B:145:PRO:HD3	2.40	0.62
1:A:53:ARG:NH1	1:A:75:ASN:O	2.33	0.62
1:A:96:LYS:HE2	5:A:546:HOH:O	1.99	0.61
1:A:154:VAL:O	1:B:18:LYS:NZ	2.33	0.59
1:A:5:LEU:HD22	1:A:220:LEU:HD23	1.84	0.58
4:A:501:GOL:H12	1:B:126:ARG:HB2	1.85	0.58
1:A:153:TYR:CE2	1:B:18:LYS:HE2	2.39	0.57
1:B:234:ARG:O	1:B:236:PRO:HD3	2.05	0.56
1:A:82:GLU:HG2	1:A:83:TRP:NE1	2.20	0.55
1:A:20:ASP:HB2	1:B:126:ARG:HH22	1.71	0.55
1:B:21:ARG:NH1	4:B:502:GOL:H31	2.21	0.54
1:B:52:LEU:HD22	1:B:249:ILE:CG2	2.38	0.54
1:B:190:GLN:HE22	1:B:232:ILE:HG21	1.72	0.54
1:A:20:ASP:HB2	1:B:126:ARG:NH2	2.23	0.53
1:B:171:PHE:CE2	1:B:260:ALA:HB2	2.44	0.53
1:B:222:ARG:HB3	1:B:255:HIS:CE1	2.44	0.52
1:B:103:THR:HB	1:B:104:PRO:CD	2.39	0.52
1:B:53:ARG:NH1	1:B:75:ASN:O	2.42	0.51
1:B:99:ARG:HH11	1:B:99:ARG:HG3	1.76	0.51
4:A:501:GOL:H12	1:B:126:ARG:HD2	1.92	0.51
1:A:255:HIS:HB3	1:A:256:PRO:CD	2.41	0.50
1:A:35:ARG:HD3	1:A:198:ASP:OD2	2.11	0.50
1:B:83:TRP:CE2	3:B:402:TP2:S1	3.05	0.49
1:B:63:LEU:O	1:B:99:ARG:NH1	2.45	0.49
1:B:225:ARG:HB3	1:B:226:PRO:HD2	1.94	0.49
1:A:83:TRP:CD2	3:A:401:TP2:S1	3.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLU:HG3	1:B:83:TRP:CZ3	2.48	0.48
1:A:116:LEU:HD12	1:A:188:MET:HE3	1.94	0.48
1:A:153:TYR:CZ	1:B:18:LYS:HE2	2.48	0.48
1:B:225:ARG:HG2	1:B:225:ARG:HH11	1.77	0.48
1:A:225:ARG:HB3	1:A:226:PRO:CD	2.44	0.47
1:A:18:LYS:HB3	5:A:625:HOH:O	2.14	0.47
1:B:3[A]:GLN:HG2	5:B:627:HOH:O	2.14	0.47
1:A:116:LEU:HD12	1:A:188:MET:CE	2.45	0.47
1:A:255:HIS:HB3	1:A:256:PRO:HD2	1.96	0.47
1:B:3[A]:GLN:CG	5:B:627:HOH:O	2.61	0.46
1:B:77:VAL:HA	5:B:596:HOH:O	2.16	0.46
1:B:129:ILE:HD13	1:B:149:PHE:CZ	2.51	0.46
1:A:2:LYS:HE3	1:A:6:GLU:OE2	2.16	0.46
1:B:99:ARG:NH1	1:B:99:ARG:HG3	2.32	0.45
1:A:22:THR:HG21	1:A:264:ILE:HG13	1.98	0.45
1:B:52:LEU:HA	1:B:55:ILE:HD12	1.98	0.45
1:A:52:LEU:HD22	1:A:249:ILE:HG13	1.98	0.45
1:A:83:TRP:CE2	3:A:401:TP2:S1	3.10	0.44
1:A:20:ASP:CB	1:B:126:ARG:HH22	2.29	0.43
1:A:126:ARG:HH11	4:B:502:GOL:H12	1.83	0.43
1:A:260:ALA:HB1	1:A:261:PRO:HD2	2.00	0.43
1:B:44:LEU:HD22	1:B:52:LEU:HD13	2.01	0.43
1:A:225:ARG:HB3	1:A:226:PRO:HD2	2.00	0.43
1:B:124:ASP:O	1:B:125:SER:C	2.57	0.42
1:A:22:THR:HG21	1:A:264:ILE:CD1	2.48	0.42
1:A:126:ARG:HD3	4:B:502:GOL:H11	1.99	0.42
1:A:83:TRP:CZ2	3:A:401:TP2:HC21	2.55	0.42
1:A:20:ASP:HB2	1:B:126:ARG:CZ	2.49	0.42
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.78	0.41
1:B:70:ALA:O	1:B:74:GLU:HG3	2.20	0.41
1:A:35:ARG:HH11	1:A:35:ARG:HD3	1.67	0.41
1:B:96:LYS:HD2	1:B:100:ALA:HB3	2.03	0.41
1:A:22:THR:HG21	1:A:264:ILE:HD11	2.03	0.40
1:B:48:LYS:HB3	1:B:258:ILE:HD12	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	263/264 (100%)	255 (97%)	6 (2%)	2 (1%)	24	15
1	B	263/264 (100%)	250 (95%)	12 (5%)	1 (0%)	39	34
All	All	526/528 (100%)	505 (96%)	18 (3%)	3 (1%)	30	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	B	94	TYR
1	A	228	PRO

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	233/232 (100%)	224 (96%)	9 (4%)	39	36
1	B	233/232 (100%)	222 (95%)	11 (5%)	32	28
All	All	466/464 (100%)	446 (96%)	20 (4%)	35	32

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

Mol	Chain	Res	Type
1	A	14	GLU
1	A	20	ASP
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	116	LEU
1	A	126	ARG
1	A	163	LEU
1	A	188	MET
1	A	229	LYS
1	A	237	GLU
1	B	18	LYS
1	B	43	PRO
1	B	76	ASN
1	B	102	PRO
1	B	115	VAL
1	B	116	LEU
1	B	146	SER
1	B	149	PHE
1	B	166	ARG
1	B	237	GLU
1	B	256	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	219	GLN
1	B	73	HIS
1	B	190	GLN
1	B	219	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CXM	A	1	1	6,10,11	1.61	2 (33%)	4,11,13	1.50	1 (25%)
1	CXM	B	1	1	6,10,11	2.09	1 (16%)	4,11,13	1.59	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	A	1	1	-	0/6/10/12	0/0/0/0
1	CXM	B	1	1	-	0/6/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	CXM	CA-N	-4.51	1.39	1.46
1	A	1	CXM	CA-N	-2.74	1.42	1.46
1	A	1	CXM	O-C	2.10	1.29	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	CXM	O-C-CA	-2.94	117.68	125.44
1	B	1	CXM	O-C-CA	-2.89	117.80	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	TP2	A	401	1	22,22,22	4.42	3 (13%)	30,31,31	2.67	10 (33%)
4	GOL	A	501	-	5,5,5	0.82	0	5,5,5	1.34	1 (20%)
2	SO4	A	511	-	4,4,4	0.93	0	6,6,6	0.48	0
2	SO4	A	512	-	4,4,4	0.96	0	6,6,6	1.11	1 (16%)
3	TP2	B	402	1	22,22,22	4.19	3 (13%)	30,31,31	1.93	10 (33%)
4	GOL	B	502	-	5,5,5	0.62	0	5,5,5	2.64	3 (60%)
2	SO4	B	513	-	4,4,4	0.82	0	6,6,6	0.62	0
2	SO4	B	514	-	4,4,4	0.71	0	6,6,6	0.62	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	TP2	A	401	1	-	0/20/30/30	0/2/2/2
4	GOL	A	501	-	-	0/4/4/4	0/0/0/0
2	SO4	A	511	-	-	0/0/0/0	0/0/0/0
2	SO4	A	512	-	-	0/0/0/0	0/0/0/0
3	TP2	B	402	1	-	0/20/30/30	0/2/2/2
4	GOL	B	502	-	-	0/4/4/4	0/0/0/0
2	SO4	B	513	-	-	0/0/0/0	0/0/0/0
2	SO4	B	514	-	-	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	401	TP2	S8-N7	10.08	1.78	1.63
3	B	402	TP2	S8-N7	10.33	1.78	1.63
3	B	402	TP2	O17-S8	11.29	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	TP2	O17-S8	11.52	1.58	1.43
3	B	402	TP2	O16-S8	11.99	1.58	1.43
3	A	401	TP2	O16-S8	13.69	1.60	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	TP2	O17-S8-O16	-7.00	107.39	119.47
3	B	402	TP2	O17-S8-O16	-5.37	110.20	119.47
3	A	401	TP2	C6-N7-S8	-3.79	112.12	119.85
4	B	502	GOL	O1-C1-C2	-3.61	92.69	110.18
4	B	502	GOL	O2-C2-C1	-3.52	92.49	108.65
3	A	401	TP2	O16-S8-N7	-3.24	100.09	106.97
3	B	402	TP2	C10-C9-S8	-2.88	116.61	119.79
3	B	402	TP2	C18-N7-S8	-2.70	112.52	119.58
3	B	402	TP2	O21-C5-C6	-2.41	114.97	120.51
3	A	401	TP2	C18-N7-S8	-2.16	113.95	119.58
3	B	402	TP2	C6-N7-S8	-2.16	115.45	119.85
3	A	401	TP2	C3-N4-C5	-2.14	118.29	122.53
3	B	402	TP2	O17-S8-C9	2.16	110.81	108.00
2	A	512	SO4	O4-S-O3	2.23	118.04	108.98
4	A	501	GOL	O3-C3-C2	2.25	121.10	110.18
3	B	402	TP2	C5-C6-N7	2.44	115.92	110.72
3	B	402	TP2	O21-C5-N4	2.52	128.13	123.08
3	A	401	TP2	O16-S8-C9	2.60	111.38	108.00
3	B	402	TP2	C14-C9-S8	2.64	122.70	119.79
4	B	502	GOL	O3-C3-C2	2.83	123.89	110.18
3	A	401	TP2	C10-C9-S8	3.14	123.25	119.79
3	A	401	TP2	C9-S8-N7	3.76	113.53	107.38
3	B	402	TP2	O16-S8-C9	4.71	114.12	108.00
3	A	401	TP2	C20-C6-C5	5.34	121.07	111.26
3	A	401	TP2	O17-S8-C9	7.13	117.26	108.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	TP2	3	0
4	A	501	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	TP2	1	0
4	B	502	GOL	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.