Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 09:29 pm GMT

PDB ID	:	4UBW
Title	:	Apo structure of the 3-ketoacyl-CoA thiolase FadA5 from M. tuberculosis
Authors	:	Schaefer, C.M.; Kisker, C.
Deposited on	:	2014-08-13
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

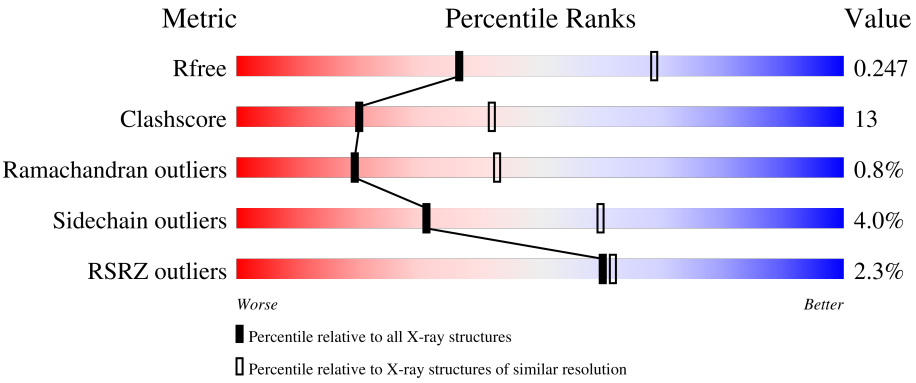
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	399	4% 71% 23%
1	B	399	% 78% 19%

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
2	GOL	B	402	-	-	X	-
3	DMS	A	406	-	-	-	X
3	DMS	A	411	-	-	-	X
3	DMS	A	413	-	-	-	X
3	DMS	A	418	-	-	-	X
3	DMS	A	419	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6172 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.

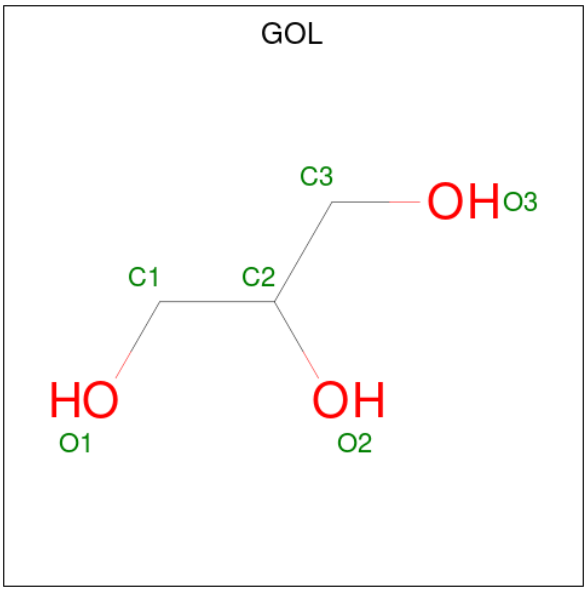
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase FadA5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	8	0
			2904	1796	542	553	13			
1	B	391	Total	C	N	O	S	0	12	0
			2965	1840	551	560	14			

There are 16 discrepancies between the modelled and reference sequences:

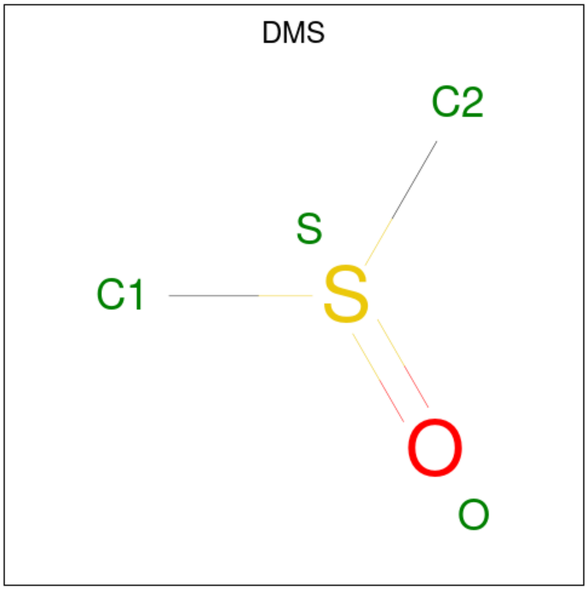
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP I6XHI4
A	-6	HIS	-	expression tag	UNP I6XHI4
A	-5	HIS	-	expression tag	UNP I6XHI4
A	-4	HIS	-	expression tag	UNP I6XHI4
A	-3	HIS	-	expression tag	UNP I6XHI4
A	-2	HIS	-	expression tag	UNP I6XHI4
A	-1	GLY	-	expression tag	UNP I6XHI4
A	0	SER	-	expression tag	UNP I6XHI4
B	-7	HIS	-	expression tag	UNP I6XHI4
B	-6	HIS	-	expression tag	UNP I6XHI4
B	-5	HIS	-	expression tag	UNP I6XHI4
B	-4	HIS	-	expression tag	UNP I6XHI4
B	-3	HIS	-	expression tag	UNP I6XHI4
B	-2	HIS	-	expression tag	UNP I6XHI4
B	-1	GLY	-	expression tag	UNP I6XHI4
B	0	SER	-	expression tag	UNP I6XHI4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	83	Total O 83 83	0	0

Continued on next page...

Continued from previous page...

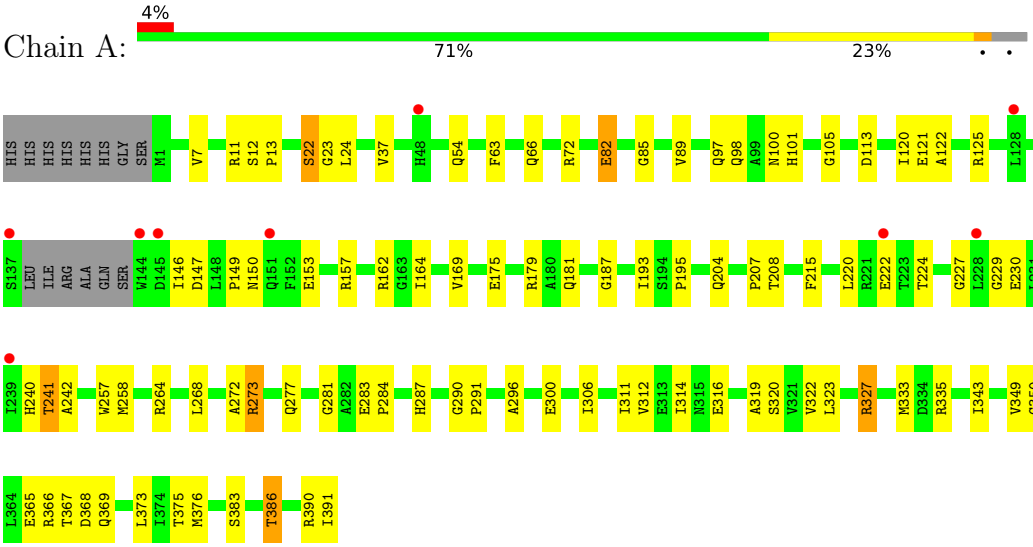
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	78	Total O 78 78	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

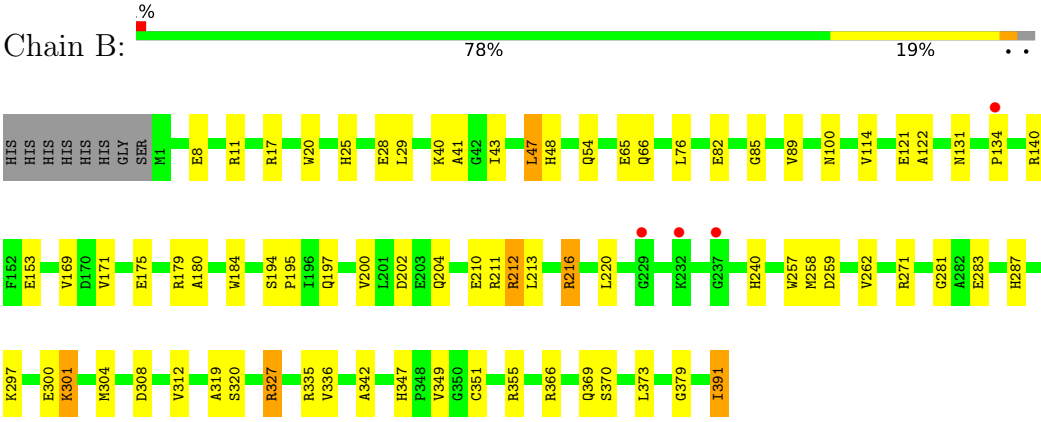
• Molecule 1: Acetyl-CoA acetyltransferase FadA5

Chain A:



• Molecule 1: Acetyl-CoA acetyltransferase FadA5

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.25Å 128.25Å 114.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.29 – 2.70 51.24 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.7 (51.29-2.70) 93.9 (51.24-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.171 , 0.248 0.171 , 0.247	Depositor DCC
R_{free} test set	1264 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6172	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 35.63 % 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 5.6667e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, DMS, CL

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	0.61	0/2962	0.85	2/4014 (0.0%)
1	B	0.61	0/3040	0.78	1/4118 (0.0%)
All	All	0.61	0/6002	0.81	3/8132 (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(^{o})	Ideal(^{o})
1	A	273	ARG	NE-CZ-NH2	5.43	123.01	120.30
1	B	17	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	72	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241[A]	THR	Peptide

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	2904	0	2906	82	0
1	B	2965	0	2989	74	0
2	A	24	0	32	3	0
2	B	12	0	16	6	0
3	A	68	0	102	5	0
3	B	36	0	54	2	0
4	B	1	0	0	0	0
5	B	1	0	0	0	0
6	A	83	0	0	4	0
6	B	78	0	0	7	0
All	All	6172	0	6099	152	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 13.

All (152) 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)
3:A:419:DMS:S	3:A:419:DMS:C1	2.13	1.34
1:A:327[A]:ARG:HH11	1:A:327[A]:ARG:HG3	1.05	1.12
1:B:370[B]:SER:OG	6:B:501:HOH:O	1.74	1.04
1:A:327[A]:ARG:HH11	1:A:327[A]:ARG:CG	1.72	1.03
1:B:47:LEU:HD13	1:B:258:MET:HE1	1.44	0.99
1:B:271[B]:ARG:CG	1:B:271[B]:ARG:HH11	1.76	0.99
1:A:7:VAL:HG21	1:A:258:MET:HE2	1.48	0.94
1:A:7:VAL:HG21	1:A:258:MET:CE	1.98	0.94
1:B:271[B]:ARG:HH11	1:B:271[B]:ARG:HG2	1.33	0.91
1:A:327[A]:ARG:HG3	1:A:327[A]:ARG:NH1	1.73	0.89
1:B:48[B]:HIS:ND1	6:B:502:HOH:O	2.08	0.85
1:B:66:GLN:NE2	1:B:122:ALA:H	1.79	0.80
1:A:258:MET:CE	1:A:268:LEU:HD22	2.12	0.79
1:B:295:THR:HG23	1:B:373:LEU:HD21	1.63	0.79
1:B:175:GLU:HG2	2:B:401:GOL:H31	1.62	0.78
1:A:66:GLN:HE22	1:A:122:ALA:H	1.33	0.77
1:A:240:HIS:HE1	1:A:320:SER:H	1.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:HB3	1:A:343:ILE:HD12	1.69	0.75
1:B:297:LYS:HE3	1:B:301[B]:LYS:HE3	1.69	0.74
1:A:335:ARG:HH12	1:A:369:GLN:HE22	1.34	0.74
1:A:258:MET:HE1	1:A:268:LEU:HD22	1.71	0.72
1:B:171:VAL:HG12	2:B:401:GOL:H11	1.72	0.71
1:B:100:ASN:HD22	1:B:257:TRP:HE1	1.39	0.71
1:B:47:LEU:HD13	1:B:258:MET:CE	2.21	0.71
1:B:66:GLN:HE22	1:B:122:ALA:H	1.36	0.71
1:B:202:ASP:O	1:B:204:GLN:O	2.10	0.70
1:B:259:ASP:HB3	1:B:262[B]:VAL:HG22	1.73	0.70
1:B:197:GLN:HG2	1:B:211:ARG:HE	1.58	0.69
1:B:100:ASN:ND2	1:B:257:TRP:HE1	1.91	0.67
1:A:373:LEU:HD12	1:A:386:THR:O	1.93	0.67
1:A:66:GLN:NE2	1:A:122:ALA:H	1.95	0.64
1:A:314:ILE:HG13	1:A:375:THR:HG23	1.78	0.64
1:B:20:TRP:HE1	2:B:402:GOL:H2	1.63	0.63
1:A:258:MET:HE3	1:A:268:LEU:HD22	1.80	0.63
1:A:240:HIS:CE1	1:A:320:SER:H	2.17	0.62
1:B:197:GLN:HG2	1:B:211:ARG:HH21	1.64	0.62
1:B:271[B]:ARG:HH11	1:B:271[B]:ARG:HG3	1.62	0.61
1:A:335:ARG:HH12	1:A:369:GLN:NE2	1.96	0.61
1:A:24:LEU:O	1:A:125[B]:ARG:HD2	2.01	0.61
1:A:100:ASN:HD22	1:A:257:TRP:HE1	1.47	0.60
1:B:271[B]:ARG:HG2	1:B:271[B]:ARG:NH1	2.11	0.60
1:B:8[A]:GLU:HG3	1:B:41:ALA:HB2	1.84	0.59
1:A:121:GLU:HG2	1:A:349:VAL:HG22	1.85	0.59
1:B:175:GLU:O	1:B:179:ARG:HG3	2.02	0.59
1:A:314:ILE:HG21	1:A:322:VAL:HG13	1.85	0.59
1:A:146:ILE:HG13	1:A:147:ASP:H	1.67	0.58
1:B:366:ARG:HG2	1:B:366:ARG:O	2.02	0.58
1:B:212[A]:ARG:HG3	1:B:213:LEU:N	2.18	0.58
1:B:76:LEU:CD2	1:B:82[B]:GLU:HG3	2.34	0.57
1:A:227:GLY:HA3	3:A:414:DMS:H23	1.87	0.57
1:B:366:ARG:O	1:B:366:ARG:CG	2.52	0.57
1:B:25:HIS:CE1	1:B:65:GLU:HG2	2.39	0.57
1:B:184:TRP:CH2	1:B:216:ARG:HA	2.39	0.57
1:A:7:VAL:CG2	1:A:258:MET:HE2	2.29	0.56
1:B:327[A]:ARG:NH1	6:B:503:HOH:O	2.26	0.56
1:A:121:GLU:HB2	1:A:350:GLY:H	1.70	0.56
1:A:290:GLY:HA3	1:A:383:SER:HB2	1.87	0.56
1:A:120:ILE:HG13	1:A:121:GLU:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:O	1:A:390:ARG:NH1	2.39	0.56
1:A:391:ILE:CG2	1:A:391:ILE:O	2.53	0.56
1:A:162:ARG:HB2	1:A:164:ILE:HG13	1.88	0.55
1:B:200:VAL:HG23	1:B:210:GLU:O	2.06	0.55
1:A:306:ILE:O	3:A:408:DMS:H23	2.08	0.54
1:B:335:ARG:HH12	1:B:369:GLN:HE22	1.56	0.54
1:A:367:THR:HG21	6:A:524:HOH:O	2.07	0.54
1:A:175:GLU:HG3	1:A:179:ARG:HD2	1.90	0.53
1:A:312:VAL:HG22	1:A:373:LEU:HB3	1.90	0.53
1:A:7:VAL:HG21	1:A:258:MET:HE3	1.89	0.53
1:A:181:GLN:HG2	1:A:220:LEU:HD23	1.90	0.53
1:A:153:GLU:O	1:A:157:ARG:HG3	2.08	0.53
1:B:11:ARG:HD3	1:B:355:ARG:HG2	1.91	0.52
1:B:25:HIS:HB2	1:B:28:GLU:OE1	2.09	0.52
1:B:212[A]:ARG:HH12	2:B:402:GOL:H12	1.74	0.52
1:B:271[B]:ARG:CG	1:B:271[B]:ARG:NH1	2.48	0.52
1:B:312:VAL:HB	1:B:336:VAL:HG22	1.92	0.52
1:A:323:LEU:HD22	2:A:402:GOL:H11	1.91	0.51
1:A:283:GLU:HG3	6:A:529:HOH:O	2.11	0.51
1:A:390:ARG:HB3	1:A:390:ARG:HH11	1.75	0.51
1:A:195:PRO:HB3	1:A:215:PHE:HB3	1.91	0.51
1:A:365:GLU:HG3	1:A:390:ARG:HD2	1.93	0.51
1:B:140:ARG:O	1:B:141:ALA:CB	2.58	0.51
1:A:105:GLY:HA3	6:B:554:HOH:O	2.10	0.51
1:A:327[A]:ARG:CG	1:A:327[A]:ARG:NH1	2.44	0.50
1:A:284:PRO:HG3	1:B:82[B]:GLU:HG2	1.94	0.50
1:B:197:GLN:HG2	1:B:211:ARG:NE	2.26	0.49
1:A:150:ASN:OD1	1:A:153:GLU:HG3	2.12	0.49
1:B:342:ALA:HB1	1:B:347:HIS:HB2	1.95	0.49
1:A:327[A]:ARG:HG2	2:A:402:GOL:H31	1.95	0.48
1:B:29:LEU:HD12	1:B:29:LEU:O	2.13	0.48
1:A:100:ASN:ND2	1:A:257:TRP:HE1	2.10	0.48
1:A:187:GLY:HA2	6:A:525:HOH:O	2.12	0.48
1:B:391:ILE:HD12	1:B:391:ILE:HA	1.75	0.48
1:B:47:LEU:CD1	1:B:258:MET:CE	2.90	0.47
1:B:169:VAL:HB	1:B:319:ALA:HB3	1.95	0.47
1:A:169:VAL:HB	1:A:319:ALA:HB3	1.96	0.47
1:A:273:ARG:HD2	6:A:554:HOH:O	2.14	0.47
1:A:296:ALA:O	1:A:300:GLU:HB2	2.14	0.47
1:B:287:HIS:NE2	1:B:379:GLY:HA2	2.29	0.47
1:A:97:GLN:OE1	1:A:376:MET:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLN:HG2	1:B:211:ARG:NH2	2.29	0.46
1:A:164:ILE:HD13	1:A:323:LEU:HB2	1.97	0.46
1:A:113:ASP:O	1:A:258:MET:HA	2.16	0.46
1:A:101:HIS:HB3	1:A:277:GLN:OE1	2.16	0.46
1:B:197:GLN:CG	1:B:211:ARG:HE	2.28	0.46
1:A:98:GLN:HA	1:A:98:GLN:OE1	2.16	0.45
1:A:181:GLN:CG	1:A:220:LEU:HD23	2.46	0.45
1:A:316:GLU:CB	1:A:343:ILE:HD12	2.44	0.45
1:B:347:HIS:CE1	1:B:349:VAL:HA	2.52	0.45
1:A:82:GLU:O	1:B:281:GLY:HA3	2.17	0.44
1:A:363:GLU:OE2	1:A:366:ARG:NH2	2.33	0.44
1:B:271[B]:ARG:HG3	1:B:271[B]:ARG:NH1	2.25	0.44
1:A:63:PHE:CD1	1:B:131:ASN:O	2.70	0.44
1:B:184:TRP:CZ2	1:B:216:ARG:HA	2.53	0.44
1:A:13:PRO:HD3	1:A:193:ILE:HG23	2.00	0.44
1:A:284:PRO:CG	1:B:82[B]:GLU:HG2	2.48	0.44
1:B:114:VAL:HG22	1:B:258:MET:HG2	1.99	0.44
1:B:140:ARG:O	1:B:141:ALA:HB3	2.18	0.44
1:B:8[B]:GLU:HG2	1:B:40[B]:LYS:HB3	1.99	0.44
1:B:29:LEU:HD12	1:B:29:LEU:C	2.37	0.44
1:B:54:GLN:HA	1:B:85:GLY:O	2.18	0.44
1:B:212[A]:ARG:HH22	2:B:402:GOL:H32	1.83	0.44
1:B:151:GLN:HG3	6:B:555:HOH:O	2.17	0.43
1:B:180:ALA:HB1	1:B:220:LEU:HD11	2.00	0.43
1:A:54:GLN:HA	1:A:85:GLY:O	2.18	0.43
1:B:8[B]:GLU:OE2	1:B:40[B]:LYS:HD3	2.19	0.43
1:B:153:GLU:HG2	6:B:536:HOH:O	2.18	0.43
1:A:311:ILE:HD13	1:A:311:ILE:HA	1.77	0.43
1:B:304:MET:HB3	1:B:308:ASP:OD2	2.18	0.43
1:A:98:GLN:OE1	1:A:101:HIS:HB2	2.19	0.43
1:B:194:SER:HA	1:B:195:PRO:HD3	1.82	0.43
1:A:207:PRO:C	1:A:208:THR:O	2.58	0.42
1:B:240:HIS:HE1	1:B:320:SER:H	1.66	0.42
1:A:11:ARG:HG3	1:A:12:SER:O	2.20	0.42
1:A:232:LYS:C	1:A:241[B]:THR:HG22	2.41	0.42
1:A:23:GLY:HA2	1:A:125[B]:ARG:HH11	1.85	0.42
1:A:241[B]:THR:O	1:A:242:ALA:HB3	2.19	0.42
1:B:212[A]:ARG:NH1	2:B:402:GOL:H12	2.35	0.42
1:A:125[B]:ARG:O	2:A:401:GOL:O2	2.37	0.41
1:A:22:SER:HB2	3:A:409:DMS:O	2.20	0.41
1:A:272:ALA:HB2	1:A:361:LEU:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLU:H	1:B:283:GLU:HG3	1.60	0.41
1:A:391:ILE:O	1:A:391:ILE:HG22	2.20	0.41
1:B:40[A]:LYS:HE2	6:B:523:HOH:O	2.20	0.41
1:B:66:GLN:HE22	1:B:121:GLU:HA	1.85	0.41
1:A:89:VAL:HG12	1:B:89:VAL:HG12	2.03	0.40
1:A:149:PRO:HG2	1:A:287:HIS:HB2	2.03	0.40
1:B:20:TRP:CD2	3:B:403:DMS:H21	2.56	0.40
1:B:212[A]:ARG:NH2	3:B:403:DMS:H22	2.37	0.40
1:A:22:SER:O	1:A:125[B]:ARG:NE	2.55	0.40
1:A:224:THR:H	3:A:414:DMS:C2	2.35	0.40
1:A:335:ARG:NH1	1:A:369:GLN:HE22	2.11	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	389/399 (98%)	359 (92%)	27 (7%)	3 (1%)	19	43
1	B	400/399 (100%)	376 (94%)	21 (5%)	3 (1%)	19	43
All	All	789/798 (99%)	735 (93%)	48 (6%)	6 (1%)	19	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ASP
1	A	136	ARG
1	A	229	GLY
1	B	141	ALA
1	B	134	PRO
1	B	290	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	297/303 (98%)	283 (95%)	14 (5%)	26	54
1	B	304/303 (100%)	291 (96%)	13 (4%)	29	57
All	All	601/606 (99%)	574 (96%)	27 (4%)	31	55

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	37	VAL
1	A	82	GLU
1	A	204	GLN
1	A	222	GLU
1	A	230	GLU
1	A	232	LYS
1	A	264	ARG
1	A	291	PRO
1	A	327[A]	ARG
1	A	327[B]	ARG
1	A	333	MET
1	A	368	ASP
1	A	386	THR
1	B	43	ILE
1	B	47	LEU
1	B	142	GLN
1	B	212[A]	ARG
1	B	212[B]	ARG
1	B	216	ARG
1	B	300	GLU
1	B	301[A]	LYS
1	B	301[B]	LYS
1	B	327[A]	ARG
1	B	327[B]	ARG
1	B	351	CYS
1	B	391	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	100	ASN
1	A	240	HIS
1	A	266	HIS
1	A	369	GLN
1	B	66	GLN
1	B	68	ASN
1	B	100	ASN
1	B	150	ASN
1	B	266	HIS
1	B	369	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
3	DMS	B	403	-	3,3,3	2.06	2 (66%)	3,3,3	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DMS	A	406	-	3,3,3	2.30	2 (66%)	3,3,3	0.26	0
3	DMS	A	420	-	3,3,3	2.38	2 (66%)	3,3,3	0.37	0
2	GOL	B	402	-	5,5,5	0.38	0	5,5,5	0.34	0
3	DMS	A	411	-	3,3,3	2.36	2 (66%)	3,3,3	0.31	0
3	DMS	B	406	-	3,3,3	2.29	2 (66%)	3,3,3	0.27	0
3	DMS	A	408	-	3,3,3	2.09	2 (66%)	3,3,3	0.90	0
2	GOL	A	402	-	5,5,5	0.50	0	5,5,5	0.24	0
3	DMS	B	408	-	3,3,3	2.29	2 (66%)	3,3,3	0.46	0
2	GOL	B	401	-	5,5,5	0.99	0	5,5,5	0.53	0
3	DMS	B	411	-	3,3,3	2.32	2 (66%)	3,3,3	0.39	0
3	DMS	A	414	-	3,3,3	2.19	2 (66%)	3,3,3	0.51	0
3	DMS	B	405	-	3,3,3	2.26	2 (66%)	3,3,3	0.40	0
3	DMS	A	407	-	3,3,3	2.20	2 (66%)	3,3,3	0.45	0
3	DMS	B	410	-	3,3,3	2.42	2 (66%)	3,3,3	0.44	0
3	DMS	A	412	-	3,3,3	2.29	2 (66%)	3,3,3	0.15	0
3	DMS	A	416	-	3,3,3	2.33	2 (66%)	3,3,3	0.41	0
3	DMS	A	417	-	3,3,3	2.25	2 (66%)	3,3,3	0.21	0
3	DMS	A	419	-	3,3,3	3.10	1 (33%)	3,3,3	2.07	1 (33%)
3	DMS	B	409	-	3,3,3	2.31	2 (66%)	3,3,3	0.39	0
3	DMS	B	407	-	3,3,3	2.31	2 (66%)	3,3,3	0.38	0
3	DMS	A	413	-	3,3,3	2.24	2 (66%)	3,3,3	0.09	0
3	DMS	B	404	-	3,3,3	2.20	2 (66%)	3,3,3	0.45	0
3	DMS	A	418	-	3,3,3	2.44	2 (66%)	3,3,3	0.19	0
3	DMS	A	409	-	3,3,3	2.26	2 (66%)	3,3,3	0.13	0
3	DMS	A	405	-	3,3,3	2.26	2 (66%)	3,3,3	0.64	0
3	DMS	A	410	-	3,3,3	2.31	2 (66%)	3,3,3	0.59	0
2	GOL	A	401	-	5,5,5	0.89	0	5,5,5	0.57	0
2	GOL	A	403	-	5,5,5	0.70	0	5,5,5	0.17	0
3	DMS	A	415	-	3,3,3	2.28	2 (66%)	3,3,3	0.15	0
2	GOL	A	404	-	5,5,5	0.60	0	5,5,5	0.48	0
3	DMS	A	421	-	3,3,3	2.28	2 (66%)	3,3,3	0.18	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	GOL	A	402	-	-	4/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	4/4/4/4	-
2	GOL	A	403	-	-	0/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	A	404	-	-	4/4/4/4	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	419	DMS	C1-S	5.13	2.13	1.75
3	A	418	DMS	C1-S	2.96	1.97	1.75
3	B	410	DMS	C1-S	2.96	1.97	1.75
3	A	420	DMS	C1-S	2.91	1.97	1.75
3	A	411	DMS	C2-S	2.88	1.97	1.75
3	A	418	DMS	C2-S	2.86	1.97	1.75
3	B	410	DMS	C2-S	2.86	1.97	1.75
3	A	421	DMS	C1-S	2.86	1.97	1.75
3	A	420	DMS	C2-S	2.86	1.97	1.75
3	A	415	DMS	C1-S	2.86	1.97	1.75
3	B	407	DMS	C2-S	2.85	1.97	1.75
3	A	410	DMS	C2-S	2.85	1.97	1.75
3	A	416	DMS	C1-S	2.85	1.97	1.75
3	A	412	DMS	C2-S	2.84	1.97	1.75
3	B	411	DMS	C2-S	2.84	1.96	1.75
3	A	411	DMS	C1-S	2.83	1.96	1.75
3	B	408	DMS	C1-S	2.82	1.96	1.75
3	A	405	DMS	C1-S	2.81	1.96	1.75
3	B	404	DMS	C2-S	2.80	1.96	1.75
3	A	406	DMS	C1-S	2.80	1.96	1.75
3	B	409	DMS	C1-S	2.80	1.96	1.75
3	A	416	DMS	C2-S	2.80	1.96	1.75
3	B	409	DMS	C2-S	2.79	1.96	1.75
3	B	406	DMS	C1-S	2.79	1.96	1.75
3	A	413	DMS	C2-S	2.78	1.96	1.75
3	B	405	DMS	C2-S	2.77	1.96	1.75
3	A	409	DMS	C1-S	2.77	1.96	1.75
3	B	411	DMS	C1-S	2.77	1.96	1.75
3	B	406	DMS	C2-S	2.76	1.96	1.75
3	A	410	DMS	C1-S	2.75	1.96	1.75
3	B	408	DMS	C2-S	2.75	1.96	1.75
3	B	407	DMS	C1-S	2.75	1.96	1.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	417	DMS	C1-S	2.75	1.96	1.75
3	A	406	DMS	C2-S	2.75	1.96	1.75
3	A	414	DMS	C2-S	2.75	1.96	1.75
3	A	412	DMS	C1-S	2.74	1.96	1.75
3	A	409	DMS	C2-S	2.74	1.96	1.75
3	A	407	DMS	C2-S	2.73	1.96	1.75
3	A	417	DMS	C2-S	2.72	1.96	1.75
3	B	405	DMS	C1-S	2.71	1.96	1.75
3	A	415	DMS	C2-S	2.68	1.95	1.75
3	A	421	DMS	C2-S	2.67	1.95	1.75
3	A	413	DMS	C1-S	2.66	1.95	1.75
3	A	405	DMS	C2-S	2.64	1.95	1.75
3	A	407	DMS	C1-S	2.62	1.95	1.75
3	A	408	DMS	C1-S	2.60	1.95	1.75
3	B	403	DMS	C1-S	2.56	1.94	1.75
3	A	414	DMS	C1-S	2.56	1.94	1.75
3	B	404	DMS	C1-S	2.54	1.94	1.75
3	A	408	DMS	C2-S	2.50	1.94	1.75
3	B	403	DMS	C2-S	2.33	1.93	1.75

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	419	DMS	C2-S-C1	3.29	115.36	98.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	404	GOL	O1-C1-C2-C3
2	A	404	GOL	C1-C2-C3-O3
2	B	401	GOL	C1-C2-C3-O3
2	A	404	GOL	O1-C1-C2-O2
2	A	404	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-C3
2	A	401	GOL	C1-C2-C3-O3
2	A	402	GOL	O1-C1-C2-C3
2	A	402	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	A	402	GOL	O1-C1-C2-O2
2	A	402	GOL	O2-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	401	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	DMS	2	0
2	B	402	GOL	4	0
3	A	408	DMS	1	0
2	A	402	GOL	2	0
2	B	401	GOL	2	0
3	A	414	DMS	2	0
3	A	419	DMS	1	0
3	A	409	DMS	1	0
2	A	401	GOL	1	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

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, 95^{th} 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	385/399 (96%)	-0.17	14 (3%)	42	42	21, 36, 63, 125	0
1	B	391/399 (97%)	-0.13	4 (1%)	82	83	23, 40, 75, 102	0
All	All	776/798 (97%)	-0.15	18 (2%)	60	62	21, 37, 68, 125	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	PRO	5.0
1	A	135	ASP	4.5
1	A	144	TRP	4.1
1	A	137	SER	3.6
1	A	134	PRO	3.5
1	A	236	GLU	3.0
1	A	136	ARG	3.0
1	B	237	GLY	2.8
1	B	229	GLY	2.6
1	A	239	ILE	2.5
1	A	222	GLU	2.5
1	A	133	GLY	2.3
1	A	128	LEU	2.3
1	A	228	LEU	2.2
1	B	232	LYS	2.2
1	A	48[A]	HIS	2.1
1	A	145	ASP	2.1
1	A	151	GLN	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DMS	A	418	4/4	-0.03	0.90	121,130,148,149	0
3	DMS	A	419	4/4	0.32	0.61	149,150,158,164	0
3	DMS	A	406	4/4	0.33	0.52	116,130,132,143	0
3	DMS	A	411	4/4	0.46	0.46	100,106,108,122	0
3	DMS	A	416	4/4	0.54	0.30	95,97,99,118	0
3	DMS	B	409	4/4	0.60	0.26	103,106,114,125	0
2	GOL	B	401	6/6	0.68	0.30	62,71,74,76	0
3	DMS	A	421	4/4	0.73	0.37	108,113,120,122	0
3	DMS	A	413	4/4	0.73	0.53	121,122,128,129	0
2	GOL	A	401	6/6	0.74	0.36	60,72,78,80	0
3	DMS	A	420	4/4	0.75	0.36	78,86,89,101	0
3	DMS	A	414	4/4	0.80	0.46	83,90,102,110	0
3	DMS	A	417	4/4	0.81	0.53	102,110,113,122	0
3	DMS	B	407	4/4	0.82	0.54	90,93,98,107	0
3	DMS	B	405	4/4	0.82	0.29	87,88,101,104	0
3	DMS	B	410	4/4	0.85	0.34	80,82,85,95	0
2	GOL	A	403	6/6	0.87	0.31	61,83,84,88	0
3	DMS	A	409	4/4	0.88	0.24	92,93,101,105	0
3	DMS	A	410	4/4	0.88	0.26	65,69,77,87	0
2	GOL	A	402	6/6	0.88	0.40	70,78,81,82	0
3	DMS	B	406	4/4	0.89	0.24	80,84,84,91	0
3	DMS	B	411	4/4	0.89	0.25	82,86,98,102	0
2	GOL	B	402	6/6	0.91	0.17	65,69,70,71	0
3	DMS	A	415	4/4	0.91	0.37	86,87,90,95	0
3	DMS	A	412	4/4	0.92	0.14	65,67,71,72	0
2	GOL	A	404	6/6	0.93	0.17	54,63,67,70	0
3	DMS	B	408	4/4	0.95	0.37	66,81,81,82	0
3	DMS	A	408	4/4	0.95	0.35	68,70,72,79	0
3	DMS	B	404	4/4	0.96	0.23	64,65,68,69	0
3	DMS	A	405	4/4	0.96	0.18	53,56,65,67	0
3	DMS	A	407	4/4	0.98	0.18	46,49,52,58	0
4	NA	B	412	1/1	0.98	0.20	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DMS	B	403	4/4	0.99	0.19	39,42,43,44	0
5	CL	B	413	1/1	0.99	0.16	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.