Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:34 PM GMT

PDB ID	:	1G8J
Title	:	CRYSTAL STRUCTURE ANALYSIS OF ARSENITE OXIDASE FROM ALCALIGENES FAECALIS
Authors	:	Ellis, P.J.; Conrads, T.; Hille, R.; Kuhn, P.
Deposited on	:	2000-11-17
Resolution	:	2.03 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 (1)) were used in the production of this report:

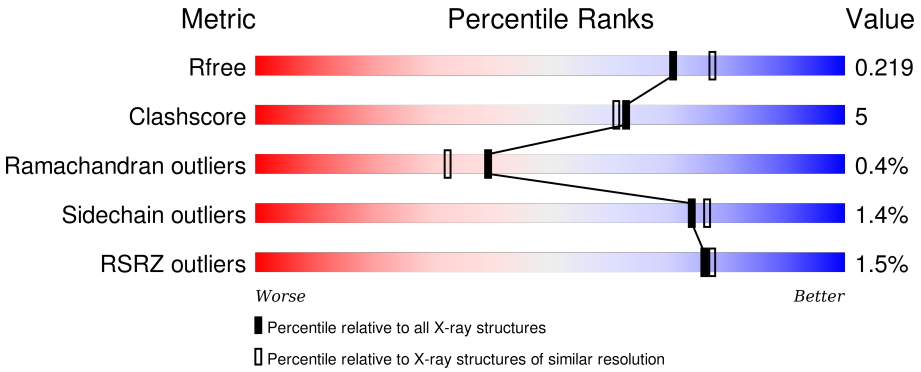
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.03 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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.

Mol	Chain	Length	Quality of chain
1	A	825	88% 11%
1	C	825	3% 86% 13%
2	B	133	2% 84% 11%
2	D	133	84% 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16253 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.

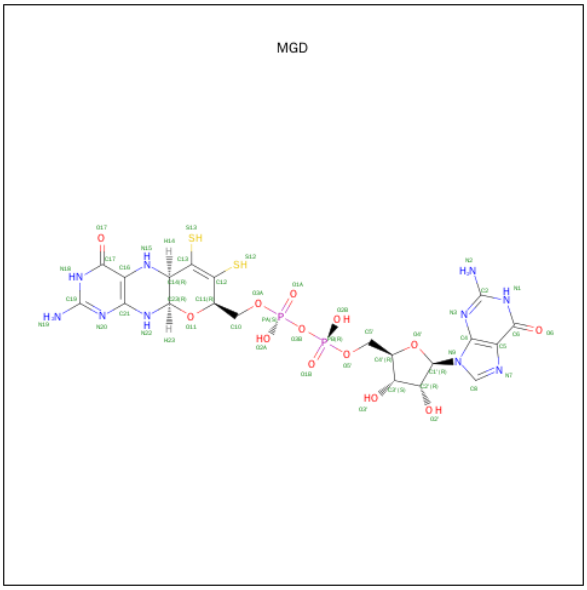
- Molecule 1 is a protein called ARSENITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C	N	O	S	149	0	0
			6435	4047	1132	1216	40			
1	C	821	Total	C	N	O	S	190	0	0
			6443	4051	1133	1219	40			

- Molecule 2 is a protein called ARSENITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	26	0	0
			926	579	150	189	8			
2	D	129	Total	C	N	O	S	21	0	0
			931	582	151	190	8			

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

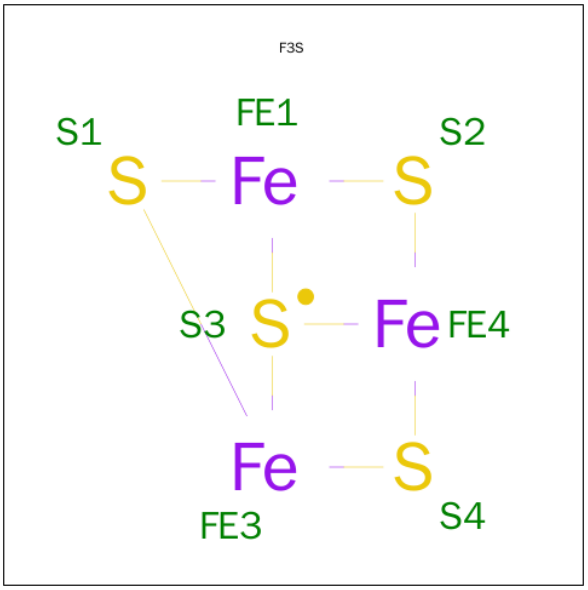
- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 5 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo).

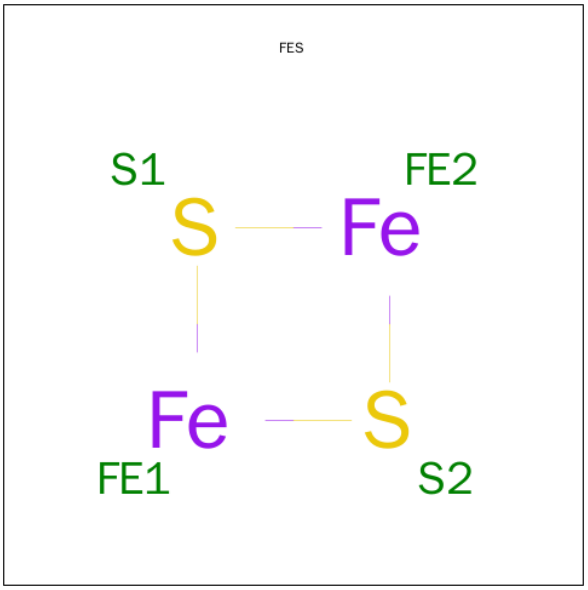
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe S 7 3 4	0	0
6	C	1	Total Fe S 7 3 4	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Fe S 4 2 2	0	0
7	D	1	Total Fe S 4 2 2	0	0

- Molecule 8 is water.

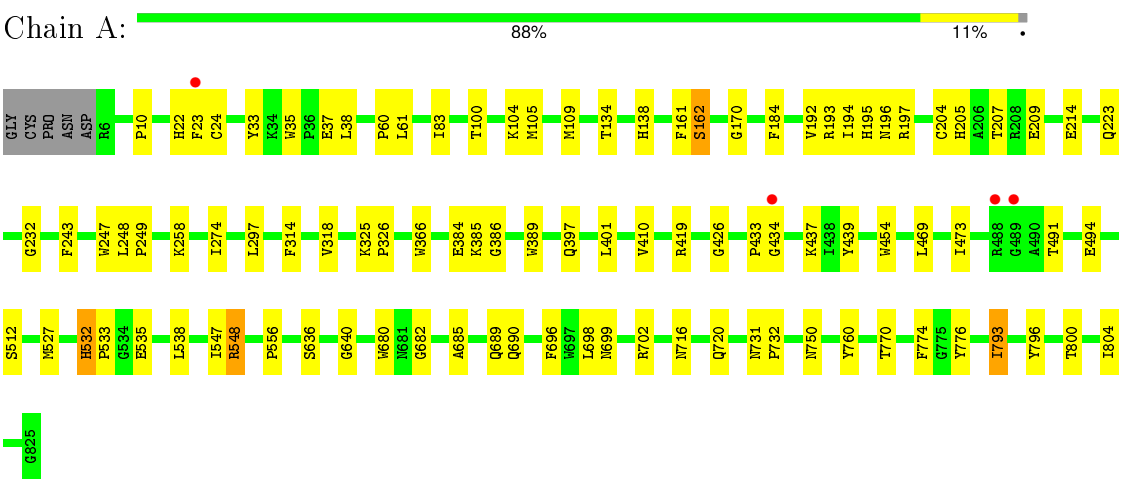
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	649	Total O 649 649	0	0
8	B	80	Total O 80 80	0	0
8	C	509	Total O 509 509	0	0
8	D	66	Total O 66 66	0	0

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.

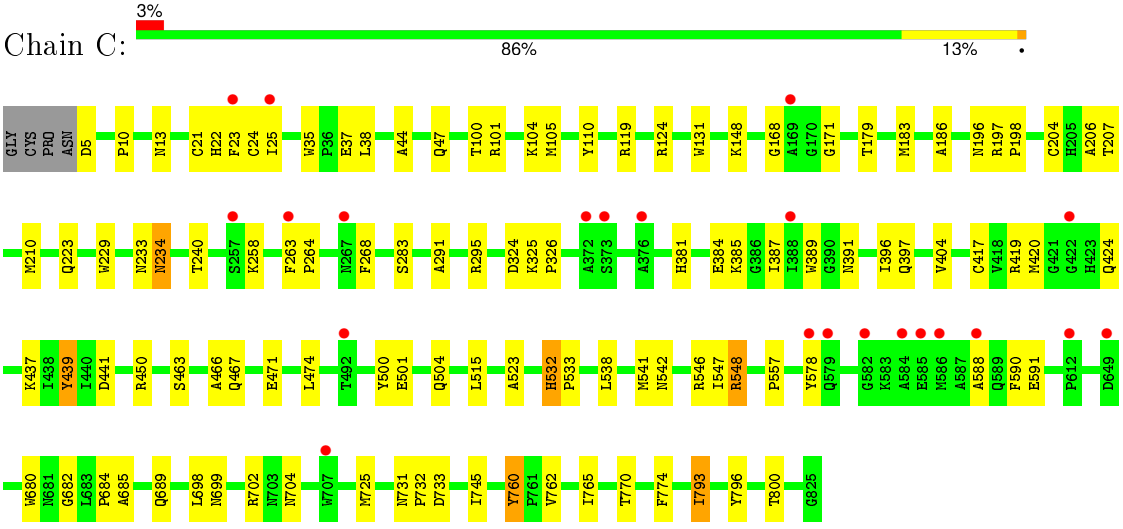
- Molecule 1: ARSENITE OXIDASE

Chain A:



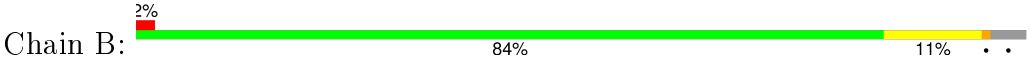
- Molecule 1: ARSENITE OXIDASE

Chain C:



- Molecule 2: ARSENITE OXIDASE

Chain B:



- Molecule 2: ARSENITE OXIDASE

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.71Å 114.25Å 108.98Å 90.00° 112.44° 90.00°	Depositor
Resolution (Å)	20.00 – 2.03 48.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.03) 91.5 (48.13-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.223 0.188 , 0.219	Depositor DCC
R_{free} test set	6563 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 135379 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16253	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 4MO, F3S, FES, O, MGD

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	0.42	0/6596	0.66	2/8942 (0.0%)
1	C	0.38	0/6604	0.63	1/8953 (0.0%)
2	B	0.36	0/947	0.65	0/1295
2	D	0.37	0/952	0.65	0/1302
All	All	0.39	0/15099	0.65	3/20492 (0.0%)

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	162	SER	N-CA-C	-5.08	97.30	111.00
1	C	23	PHE	N-CA-C	5.04	124.60	111.00
1	A	23	PHE	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6435	0	6199	57	0
1	C	6443	0	6203	71	0
2	B	926	0	884	9	0
2	D	931	0	889	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	94	0	44	3	0
3	C	94	0	45	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	1	0
6	A	7	0	0	0	0
6	C	7	0	0	0	0
7	B	4	0	0	1	0
7	D	4	0	0	1	0
8	A	649	0	0	3	0
8	B	80	0	0	1	0
8	C	509	0	0	1	0
8	D	66	0	0	1	0
All	All	16253	0	14264	147	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 (147) 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:A:698:LEU:HB2	1:A:800:THR:HG23	1.69	0.75
1:C:5:ASP:O	2:D:124:LEU:HD13	1.92	0.69
1:C:263:PHE:HB2	1:C:268:PHE:HZ	1.57	0.68
2:B:63:MET:HB2	7:B:2006:FES:S2	2.34	0.67
1:C:698:LEU:HB2	1:C:800:THR:HG23	1.77	0.67
1:C:223:GLN:HE22	1:C:258:LYS:HZ2	1.42	0.67
1:C:467:GLN:O	1:C:471:GLU:HG3	1.94	0.66
1:A:10:PRO:HB3	1:A:35:TRP:CZ3	2.32	0.65
1:C:223:GLN:HE22	1:C:258:LYS:NZ	1.93	0.65
1:C:384:GLU:HG3	1:C:385:LYS:H	1.63	0.63
3:C:3001:MGD:S13	3:C:3002:MGD:S12	2.97	0.62
1:A:384:GLU:HG3	1:A:385:LYS:H	1.64	0.61
1:C:204:CYS:HB3	1:C:207:THR:CG2	2.32	0.60
2:D:81:HIS:HB2	7:D:3006:FES:S1	2.42	0.60
1:C:186:ALA:HB1	1:C:590:PHE:CD1	2.38	0.59
1:C:391:ASN:OD1	1:C:684:PRO:HD3	2.03	0.58
2:D:12:SER:OG	2:D:13:VAL:N	2.35	0.58
1:C:110:TYR:CD2	1:C:557:PRO:HB3	2.39	0.58
1:C:22:HIS:NE2	1:C:533:PRO:HB2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ALA:HB3	1:C:47:GLN:HG3	1.85	0.58
1:A:532:HIS:HB2	1:A:533:PRO:CD	2.34	0.57
1:A:196:ASN:OD1	1:A:197:ARG:HG2	2.05	0.57
1:C:685:ALA:O	1:C:689:GLN:HG3	2.06	0.56
1:A:385:LYS:HE2	3:A:2001:MGD:S13	2.45	0.56
1:C:234:ASN:ND2	1:C:283:SER:OG	2.38	0.55
1:A:205:HIS:O	1:A:209:GLU:HG3	2.06	0.55
1:A:636:SER:OG	1:A:640:GLY:HA2	2.07	0.55
1:A:716:ASN:O	1:A:720:GLN:HG3	2.08	0.54
1:C:25:ILE:HD12	1:C:424:GLN:HA	1.89	0.54
1:C:450:ARG:NH1	1:C:504:GLN:HA	2.23	0.54
1:C:206:ALA:O	1:C:210:MET:HG3	2.07	0.53
1:A:232:GLY:HA3	1:A:386:GLY:HA3	1.90	0.53
1:C:699:ASN:HB3	1:C:770:THR:O	2.09	0.53
1:A:37:GLU:O	1:A:38:LEU:HB2	2.09	0.53
1:A:397:GLN:HG3	8:A:2088:HOH:O	2.08	0.53
1:A:274:ILE:HG12	1:A:297:LEU:HB2	1.91	0.53
1:C:223:GLN:NE2	1:C:258:LYS:NZ	2.57	0.52
1:A:100:THR:HB	2:B:97:GLU:HA	1.90	0.52
1:C:404:VAL:HG11	1:C:417:CYS:HB2	1.92	0.52
1:C:474:LEU:HD23	1:C:523:ALA:HB2	1.92	0.51
1:A:533:PRO:HG3	1:A:538:LEU:HD13	1.90	0.51
2:B:11:VAL:O	2:B:12:SER:HB2	2.11	0.51
1:C:179:THR:O	1:C:183:MET:HG3	2.10	0.51
2:D:100:ALA:HB3	8:D:3047:HOH:O	2.10	0.51
1:A:297:LEU:HG	1:A:366:TRP:CH2	2.45	0.50
1:C:21:CYS:HA	1:C:105:MET:CE	2.42	0.50
1:A:491:THR:OG1	1:A:494:GLU:HG3	2.12	0.49
1:C:324:ASP:OD2	1:C:326:PRO:HD2	2.12	0.49
1:A:699:ASN:HB3	1:A:770:THR:O	2.12	0.49
1:C:22:HIS:CD2	1:C:533:PRO:HB2	2.46	0.49
1:C:25:ILE:O	1:C:542:ASN:HB2	2.12	0.49
2:D:53:ILE:HD13	2:D:116:LEU:HD11	1.93	0.49
1:C:532:HIS:HB2	1:C:533:PRO:CD	2.43	0.48
1:C:463:SER:O	1:C:466:ALA:HB2	2.14	0.48
1:A:702:ARG:HD3	3:A:2002:MGD:H102	1.94	0.48
1:C:124:ARG:HG2	1:C:131:TRP:HE3	1.79	0.48
1:C:501:GLU:HA	1:C:504:GLN:HE21	1.79	0.47
1:C:588:ALA:HA	1:C:591:GLU:OE2	2.14	0.47
1:A:325:LYS:HB2	1:A:326:PRO:HD3	1.95	0.47
1:A:105:MET:O	1:A:109:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:GLN:OE1	1:A:750:ASN:HB2	2.15	0.47
2:D:126:TYR:CG	2:D:127:GLY:N	2.81	0.47
1:C:233:ASN:OD1	1:C:420:MET:HG3	2.14	0.47
1:A:547:ILE:O	1:A:548:ARG:HD3	2.14	0.47
1:A:469:LEU:O	1:A:473:ILE:HG12	2.14	0.47
1:C:204:CYS:HB3	1:C:207:THR:HG22	1.97	0.47
1:C:196:ASN:OD1	1:C:197:ARG:HG2	2.15	0.47
1:A:535:GLU:HB3	1:A:556:PRO:HG3	1.97	0.47
1:A:532:HIS:HB2	1:A:533:PRO:HD2	1.97	0.47
1:C:10:PRO:HB3	1:C:35:TRP:CZ3	2.50	0.47
1:A:33:TYR:O	1:A:83:ILE:HA	2.15	0.47
1:A:170:GLY:HA2	3:A:2001:MGD:C6	2.45	0.47
1:C:680:TRP:CZ2	1:C:682:GLY:HA2	2.50	0.46
3:C:3001:MGD:H13	5:C:3004:4MO:MO	1.50	0.46
1:C:541:MET:HA	1:C:546:ARG:O	2.15	0.46
1:C:731:ASN:OD1	1:C:733:ASP:HB2	2.15	0.46
1:A:204:CYS:HB3	1:A:207:THR:HG22	1.98	0.46
1:A:204:CYS:HB3	1:A:207:THR:CG2	2.45	0.46
1:C:439:TYR:CE2	1:C:441:ASP:HB2	2.50	0.46
1:C:229:TRP:HB2	1:C:381:HIS:HA	1.98	0.46
1:C:168:GLY:HA3	8:C:3061:HOH:O	2.14	0.46
2:B:18:ALA:HB3	2:B:21:GLU:HB3	1.98	0.46
1:C:437:LYS:HB3	1:C:793:ILE:HD12	1.97	0.46
2:D:83:THR:HG23	2:D:96:GLY:HA3	1.98	0.45
1:C:387:ILE:HB	1:C:396:ILE:HG21	1.99	0.45
1:C:124:ARG:HG2	1:C:131:TRP:CE3	2.52	0.45
1:C:148:LYS:HE2	1:C:578:TYR:CD1	2.51	0.45
1:C:101:ARG:NH1	1:C:704:ASN:O	2.45	0.45
1:C:37:GLU:O	1:C:38:LEU:HB2	2.17	0.45
1:A:232:GLY:CA	1:A:386:GLY:HA3	2.47	0.45
1:A:437:LYS:HA	8:A:2292:HOH:O	2.17	0.45
1:A:60:PRO:O	1:A:61:LEU:HB2	2.16	0.45
1:C:500:TYR:O	1:C:504:GLN:HG3	2.17	0.45
2:B:110:ASP:O	2:B:114:ASP:N	2.48	0.45
2:B:126:TYR:CG	2:B:127:GLY:N	2.84	0.45
1:C:119:ARG:HD2	1:C:515:LEU:O	2.17	0.45
1:C:793:ILE:O	1:C:793:ILE:HG22	2.17	0.45
1:A:214:GLU:HG3	1:A:419:ARG:HD3	1.98	0.45
2:D:18:ALA:HB3	2:D:21:GLU:HB2	1.98	0.45
1:C:148:LYS:HG3	1:C:578:TYR:CZ	2.52	0.44
1:C:702:ARG:HD3	3:C:3002:MGD:H102	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:TYR:HE2	1:C:441:ASP:HB2	1.83	0.44
1:A:434:GLY:HA3	8:A:2324:HOH:O	2.18	0.44
1:C:725:MET:SD	1:C:745:ILE:HD12	2.57	0.44
1:C:702:ARG:N	1:C:702:ARG:HD2	2.33	0.43
1:A:680:TRP:CZ2	1:A:682:GLY:HA2	2.54	0.43
1:C:450:ARG:HH12	1:C:504:GLN:HA	1.82	0.43
1:A:223:GLN:HE22	1:A:258:LYS:NZ	2.17	0.43
1:C:760:TYR:O	1:C:762:VAL:HG23	2.17	0.43
1:C:100:THR:O	1:C:104:LYS:HG3	2.19	0.43
1:C:762:VAL:HB	1:C:765:ILE:HG12	2.00	0.43
1:A:134:THR:HG1	1:A:138:HIS:HD1	1.65	0.43
1:A:243:PHE:O	1:A:247:TRP:HB2	2.19	0.43
1:C:207:THR:HG22	1:C:397:GLN:NE2	2.33	0.42
1:C:44:ALA:HB3	1:C:47:GLN:CG	2.50	0.42
1:A:793:ILE:O	1:A:793:ILE:HG22	2.19	0.42
1:A:685:ALA:O	1:A:689:GLN:HG3	2.19	0.42
2:B:38:LYS:HD3	8:B:2059:HOH:O	2.19	0.42
1:A:194:ILE:HG22	1:A:195:HIS:N	2.35	0.42
1:C:385:LYS:NZ	1:C:419:ARG:NH2	2.68	0.42
1:A:401:LEU:HD13	1:A:401:LEU:HA	1.94	0.42
1:A:314:PHE:O	1:A:318:VAL:HG23	2.20	0.42
1:A:547:ILE:C	1:A:548:ARG:HD3	2.40	0.41
1:C:171:GLY:O	1:C:538:LEU:HD11	2.19	0.41
1:A:696:PHE:CD1	1:A:804:ILE:HD12	2.55	0.41
1:A:161:PHE:HB2	1:A:192:VAL:HG22	2.03	0.41
2:B:32:SER:OG	2:B:125:ILE:HD13	2.19	0.41
1:A:297:LEU:HG	1:A:366:TRP:CZ3	2.55	0.41
1:C:124:ARG:HD3	1:C:131:TRP:HB3	2.03	0.41
1:A:248:LEU:HB2	1:A:249:PRO:HD3	2.02	0.41
1:A:22:HIS:NE2	1:A:533:PRO:HB2	2.35	0.41
1:A:100:THR:O	1:A:104:LYS:HG3	2.20	0.41
1:C:148:LYS:HE2	1:C:578:TYR:CE1	2.56	0.41
1:A:731:ASN:HA	1:A:732:PRO:HD3	1.92	0.41
1:A:162:SER:HA	1:A:193:ARG:HG3	2.01	0.41
1:C:325:LYS:HB2	1:C:326:PRO:HD3	2.02	0.41
2:D:35:VAL:HG13	2:D:58:VAL:HG11	2.02	0.41
1:A:37:GLU:HG2	1:A:38:LEU:HG	2.03	0.41
1:C:731:ASN:HA	1:C:732:PRO:HD3	1.95	0.41
1:A:702:ARG:HD2	1:A:702:ARG:N	2.36	0.41
2:D:84:GLU:HG2	2:D:94:ILE:HD12	2.02	0.41
1:A:512:SER:O	1:A:527:MET:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:GLU:HG2	2:B:94:ILE:HD12	2.03	0.40
1:C:186:ALA:HB1	1:C:590:PHE:CE1	2.56	0.40
1:C:547:ILE:C	1:C:548:ARG:HD3	2.41	0.40
1:C:291:ALA:O	1:C:295:ARG:HD3	2.20	0.40
1:A:184:PHE:CG	1:A:433:PRO:HD3	2.55	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	818/825 (99%)	785 (96%)	31 (4%)	2 (0%)	52	47
1	C	819/825 (99%)	782 (96%)	33 (4%)	4 (0%)	34	26
2	B	126/133 (95%)	120 (95%)	5 (4%)	1 (1%)	24	15
2	D	127/133 (96%)	119 (94%)	7 (6%)	1 (1%)	24	15
All	All	1890/1916 (99%)	1806 (96%)	76 (4%)	8 (0%)	39	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	PRO
2	B	12	SER
1	A	793	ILE
1	C	240	THR
2	D	12	SER
1	C	793	ILE
1	C	198	PRO
1	A	426	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	672/676 (99%)	661 (98%)	11 (2%)	70 72
1	C	673/676 (100%)	663 (98%)	10 (2%)	72 74
2	B	101/105 (96%)	100 (99%)	1 (1%)	82 85
2	D	101/105 (96%)	101 (100%)	0	100 100
All	All	1547/1562 (99%)	1525 (99%)	22 (1%)	74 76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	CYS
1	A	389	TRP
1	A	410	VAL
1	A	439	TYR
1	A	454	TRP
1	A	532	HIS
1	A	548	ARG
1	A	760	TYR
1	A	774	PHE
1	A	776	TYR
1	A	796	TYR
2	B	57	SER
1	C	13	ASN
1	C	24	CYS
1	C	234	ASN
1	C	389	TRP
1	C	439	TYR
1	C	532	HIS
1	C	548	ARG
1	C	760	TYR
1	C	774	PHE
1	C	796	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	234	ASN
1	A	397	GLN
1	A	504	GLN
1	A	579	GLN
1	A	589	GLN
1	A	689	GLN
1	A	769	GLN
1	C	223	GLN
1	C	234	ASN
1	C	397	GLN
1	C	504	GLN
1	C	579	GLN
1	C	589	GLN
1	C	689	GLN
1	C	720	GLN
1	C	769	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	MGD	A	2001	5	38,52,52	1.43	6 (15%)	43,81,81	2.57	11 (25%)
3	MGD	A	2002	5	38,52,52	1.43	5 (13%)	43,81,81	2.50	14 (32%)
6	F3S	A	2005	1	0,9,9	0.00	-	0,15,15	0.00	-
7	FES	B	2006	2	0,4,4	0.00	-	0,4,4	0.00	-
3	MGD	C	3001	5	38,52,52	1.53	6 (15%)	43,81,81	2.51	11 (25%)
3	MGD	C	3002	5	38,52,52	1.49	4 (10%)	43,81,81	2.49	14 (32%)
6	F3S	C	3005	1	0,9,9	0.00	-	0,15,15	0.00	-
7	FES	D	3006	2	0,4,4	0.00	-	0,4,4	0.00	-

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	MGD	A	2001	5	-	0/18/66/66	0/6/6/6
3	MGD	A	2002	5	-	0/18/66/66	0/6/6/6
6	F3S	A	2005	1	-	0/0/24/24	0/0/3/3
7	FES	B	2006	2	-	0/0/4/4	0/1/1/1
3	MGD	C	3001	5	-	0/18/66/66	0/6/6/6
3	MGD	C	3002	5	-	0/18/66/66	0/6/6/6
6	F3S	C	3005	1	-	0/0/24/24	0/0/3/3
7	FES	D	3006	2	-	0/0/4/4	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	MGD	C2-N1	2.00	1.38	1.35
3	C	3001	MGD	C23-N22	2.02	1.48	1.44
3	A	2001	MGD	C21-N22	2.14	1.39	1.35
3	A	2002	MGD	C21-N20	2.14	1.38	1.34
3	A	2002	MGD	C19-N18	2.22	1.39	1.35
3	A	2001	MGD	C23-N22	2.28	1.49	1.44
3	C	3001	MGD	C21-N20	2.57	1.39	1.34
3	C	3001	MGD	C19-N18	2.61	1.40	1.35
3	C	3002	MGD	C19-N18	2.64	1.40	1.35
3	A	2002	MGD	C14-N15	2.72	1.49	1.45
3	C	3002	MGD	C6-N1	3.19	1.39	1.33
3	C	3002	MGD	C21-N20	3.23	1.40	1.34
3	A	2001	MGD	C21-N20	3.29	1.40	1.34
3	A	2002	MGD	C6-N1	3.52	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	MGD	C6-N1	3.61	1.39	1.33
3	A	2001	MGD	C17-N18	3.66	1.39	1.33
3	C	3001	MGD	C6-N1	3.71	1.40	1.33
3	C	3001	MGD	C17-N18	4.07	1.40	1.33
3	C	3001	MGD	C23-C14	4.08	1.56	1.53
3	A	2002	MGD	C17-N18	4.69	1.41	1.33
3	C	3002	MGD	C17-N18	5.49	1.43	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	MGD	C5-C6-N1	-8.98	111.31	123.59
3	A	2002	MGD	C5-C6-N1	-8.88	111.44	123.59
3	C	3001	MGD	C5-C6-N1	-8.78	111.58	123.59
3	C	3002	MGD	C5-C6-N1	-8.74	111.64	123.59
3	C	3001	MGD	PA-O3B-PB	-3.77	122.14	132.73
3	C	3002	MGD	C21-N22-C23	-3.59	116.63	123.67
3	A	2001	MGD	PA-O3B-PB	-3.47	122.97	132.73
3	A	2001	MGD	N18-C19-N20	-3.25	120.21	125.53
3	A	2002	MGD	N18-C19-N20	-3.22	120.25	125.53
3	C	3001	MGD	N18-C19-N20	-3.17	120.34	125.53
3	A	2002	MGD	C4'-O4'-C1'	-3.11	106.30	109.72
3	C	3002	MGD	N18-C19-N20	-3.09	120.47	125.53
3	A	2002	MGD	C21-N22-C23	-3.00	117.80	123.67
3	C	3002	MGD	C4'-O4'-C1'	-2.93	106.50	109.72
3	A	2002	MGD	PA-O3B-PB	-2.60	125.44	132.73
3	A	2001	MGD	N3-C2-N1	-2.42	123.76	127.44
3	C	3001	MGD	N3-C2-N1	-2.37	123.83	127.44
3	A	2002	MGD	N3-C2-N1	-2.33	123.90	127.44
3	C	3002	MGD	N3-C2-N1	-2.28	123.97	127.44
3	C	3002	MGD	PA-O3B-PB	-2.26	126.39	132.73
3	C	3002	MGD	C16-C21-N22	2.07	120.51	118.34
3	A	2002	MGD	O3B-PB-O5'	2.36	109.20	102.94
3	A	2002	MGD	C16-C21-N22	2.69	121.16	118.34
3	C	3002	MGD	O3B-PB-O5'	3.02	110.96	102.94
3	C	3001	MGD	C16-C21-N22	3.14	121.63	118.34
3	C	3002	MGD	C19-N20-C21	3.30	121.95	114.54
3	C	3001	MGD	C19-N20-C21	3.38	122.14	114.54
3	A	2001	MGD	C19-N20-C21	3.41	122.19	114.54
3	A	2002	MGD	C17-C16-C21	3.42	117.66	114.56
3	A	2001	MGD	C16-C21-N22	3.43	121.94	118.34
3	A	2002	MGD	N19-C19-N20	3.49	122.98	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2002	MGD	C19-N20-C21	3.49	122.39	114.54
3	C	3001	MGD	N19-C19-N20	3.51	123.02	117.20
3	C	3001	MGD	C17-N18-C19	3.59	120.92	115.94
3	C	3002	MGD	N19-C19-N20	3.60	123.16	117.20
3	C	3002	MGD	C17-N18-C19	3.74	121.13	115.94
3	A	2002	MGD	O11-C23-C14	3.80	111.56	108.96
3	A	2002	MGD	C17-N18-C19	3.85	121.29	115.94
3	A	2001	MGD	N19-C19-N20	3.89	123.64	117.20
3	C	3002	MGD	C17-C16-C21	3.90	118.10	114.56
3	A	2001	MGD	C17-N18-C19	4.00	121.49	115.94
3	C	3002	MGD	O11-C23-C14	4.05	111.73	108.96
3	A	2001	MGD	C17-C16-C21	4.37	118.52	114.56
3	C	3001	MGD	C17-C16-C21	4.37	118.52	114.56
3	C	3001	MGD	O11-C23-C14	5.53	112.75	108.96
3	A	2001	MGD	O11-C23-C14	5.83	112.95	108.96
3	C	3001	MGD	C6-N1-C2	6.56	125.05	115.94
3	A	2001	MGD	C6-N1-C2	6.60	125.09	115.94
3	C	3002	MGD	C6-N1-C2	6.64	125.15	115.94
3	A	2002	MGD	C6-N1-C2	6.68	125.20	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	MGD	2	0
3	A	2002	MGD	1	0
7	B	2006	FES	1	0
3	C	3001	MGD	2	0
3	C	3002	MGD	2	0
7	D	3006	FES	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, 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	820/825 (99%)	-0.16	4 (0%) 91 92	12, 23, 31, 41	58 (7%)
1	C	819/825 (99%)	0.15	22 (2%) 58 59	15, 27, 38, 46	70 (8%)
2	B	128/133 (96%)	-0.04	3 (2%) 64 65	19, 28, 38, 41	9 (7%)
2	D	129/133 (96%)	0.18	0 100 100	20, 31, 43, 46	10 (7%)
All	All	1896/1916 (98%)	0.01	29 (1%) 76 77	12, 25, 37, 46	147 (7%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	584	ALA	4.6
1	A	489	GLY	4.0
1	C	263	PHE	3.8
1	C	578	TYR	3.5
1	C	586	MET	3.1
1	C	25	ILE	3.1
1	C	267	ASN	3.0
1	C	388	ILE	2.9
1	C	372	ALA	2.9
1	C	585	GLU	2.9
1	C	649	ASP	2.7
1	C	492	THR	2.6
1	C	582	GLY	2.5
1	A	488	ARG	2.4
1	C	257	SER	2.4
2	B	114	ASP	2.3
1	C	422	GLY	2.3
1	C	612	PRO	2.3
1	C	588	ALA	2.3
1	C	707	TRP	2.3
1	C	23	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	112	ALA	2.2
1	C	373	SER	2.2
1	C	376	ALA	2.2
1	A	23	PHE	2.1
1	C	169	ALA	2.1
2	B	111	ALA	2.1
1	C	579	GLN	2.1
1	A	434	GLY	2.0

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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	MGD	C	3001	47/47	0.94	0.13	-0.22	18,21,25,29	0
3	MGD	A	2001	47/47	0.95	0.14	-0.41	17,22,24,25	0
3	MGD	C	3002	47/47	0.95	0.14	-0.44	14,22,25,28	0
6	F3S	A	2005	7/7	0.82	0.12	-0.61	19,20,25,26	0
7	FES	D	3006	4/4	0.92	0.09	-0.74	26,27,32,33	0
3	MGD	A	2002	47/47	0.96	0.12	-0.80	15,19,21,24	0
6	F3S	C	3005	7/7	0.88	0.10	-1.47	22,24,30,31	0
7	FES	B	2006	4/4	0.93	0.07	-2.00	28,29,34,35	0
4	O	C	3003	1/1	0.98	0.12	-2.28	2,2,2,2	0
4	O	A	2003	1/1	0.99	0.07	-3.47	2,2,2,2	0
5	4MO	C	3004	1/1	0.99	0.05	-4.89	17,17,17,17	0
5	4MO	A	2004	1/1	0.99	0.06	-6.97	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.