Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 08:54 AM GMT

PDB ID	:	3GGS
Title	:	Human purine nucleoside phosphorylase double mutant E201Q,N243D complexed with 2-fluoro-2'-deoxyadenosine
Authors	:	Sawaya, M.R.; Afshar, S.
Deposited on	:	2009-03-02
Resolution	:	2.52 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:

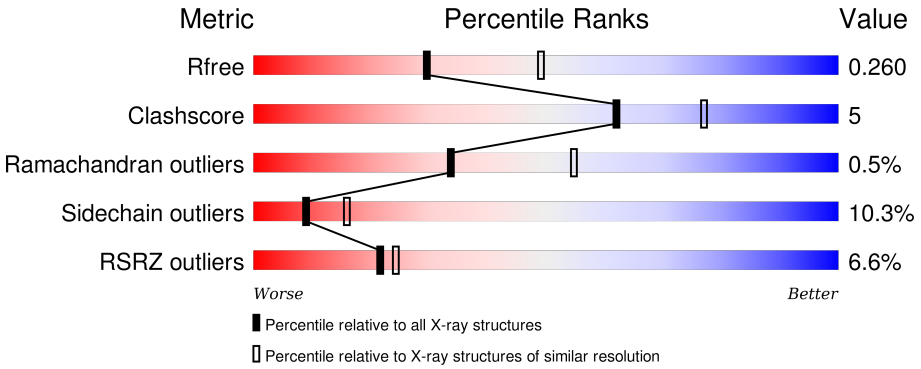
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.52 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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	311	4% 72% 18% • 9%
1	B	311	7% 78% 12% • 8%
1	C	311	7% 73% 14% • 10%

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	2FD	C	301	-	-	-	X
3	SO4	C	294	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6904 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 Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2211	1407	386	403	15			
1	B	285	Total	C	N	O	S	0	0	0
			2220	1413	387	404	16			
1	C	279	Total	C	N	O	S	0	0	0
			2183	1389	382	397	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	LYS	-	EXPRESSION TAG	UNP P00491
A	-20	GLU	-	EXPRESSION TAG	UNP P00491
A	-19	THR	-	EXPRESSION TAG	UNP P00491
A	-18	ALA	-	EXPRESSION TAG	UNP P00491
A	-17	ALA	-	EXPRESSION TAG	UNP P00491
A	-16	ALA	-	EXPRESSION TAG	UNP P00491
A	-15	LYS	-	EXPRESSION TAG	UNP P00491
A	-14	PHE	-	EXPRESSION TAG	UNP P00491
A	-13	GLU	-	EXPRESSION TAG	UNP P00491
A	-12	ARG	-	EXPRESSION TAG	UNP P00491
A	-11	GLN	-	EXPRESSION TAG	UNP P00491
A	-10	HIS	-	EXPRESSION TAG	UNP P00491
A	-9	MET	-	EXPRESSION TAG	UNP P00491
A	-8	ASP	-	EXPRESSION TAG	UNP P00491
A	-7	SER	-	EXPRESSION TAG	UNP P00491
A	-6	GLY	-	EXPRESSION TAG	UNP P00491
A	-5	GLY	-	EXPRESSION TAG	UNP P00491
A	-4	GLY	-	EXPRESSION TAG	UNP P00491
A	-3	GLY	-	EXPRESSION TAG	UNP P00491
A	-2	SER	-	EXPRESSION TAG	UNP P00491
A	-1	GLY	-	EXPRESSION TAG	UNP P00491
A	0	HIS	-	EXPRESSION TAG	UNP P00491
A	201	GLN	GLU	ENGINEERED	UNP P00491

Continued on next page...

Continued from previous page...

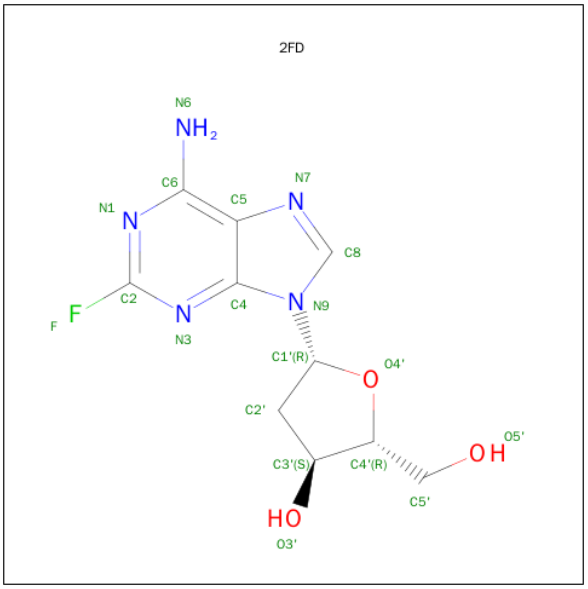
Chain	Residue	Modelled	Actual	Comment	Reference
A	243	ASP	ASN	ENGINEERED	UNP P00491
B	-21	LYS	-	EXPRESSION TAG	UNP P00491
B	-20	GLU	-	EXPRESSION TAG	UNP P00491
B	-19	THR	-	EXPRESSION TAG	UNP P00491
B	-18	ALA	-	EXPRESSION TAG	UNP P00491
B	-17	ALA	-	EXPRESSION TAG	UNP P00491
B	-16	ALA	-	EXPRESSION TAG	UNP P00491
B	-15	LYS	-	EXPRESSION TAG	UNP P00491
B	-14	PHE	-	EXPRESSION TAG	UNP P00491
B	-13	GLU	-	EXPRESSION TAG	UNP P00491
B	-12	ARG	-	EXPRESSION TAG	UNP P00491
B	-11	GLN	-	EXPRESSION TAG	UNP P00491
B	-10	HIS	-	EXPRESSION TAG	UNP P00491
B	-9	MET	-	EXPRESSION TAG	UNP P00491
B	-8	ASP	-	EXPRESSION TAG	UNP P00491
B	-7	SER	-	EXPRESSION TAG	UNP P00491
B	-6	GLY	-	EXPRESSION TAG	UNP P00491
B	-5	GLY	-	EXPRESSION TAG	UNP P00491
B	-4	GLY	-	EXPRESSION TAG	UNP P00491
B	-3	GLY	-	EXPRESSION TAG	UNP P00491
B	-2	SER	-	EXPRESSION TAG	UNP P00491
B	-1	GLY	-	EXPRESSION TAG	UNP P00491
B	0	HIS	-	EXPRESSION TAG	UNP P00491
B	201	GLN	GLU	ENGINEERED	UNP P00491
B	243	ASP	ASN	ENGINEERED	UNP P00491
C	-21	LYS	-	EXPRESSION TAG	UNP P00491
C	-20	GLU	-	EXPRESSION TAG	UNP P00491
C	-19	THR	-	EXPRESSION TAG	UNP P00491
C	-18	ALA	-	EXPRESSION TAG	UNP P00491
C	-17	ALA	-	EXPRESSION TAG	UNP P00491
C	-16	ALA	-	EXPRESSION TAG	UNP P00491
C	-15	LYS	-	EXPRESSION TAG	UNP P00491
C	-14	PHE	-	EXPRESSION TAG	UNP P00491
C	-13	GLU	-	EXPRESSION TAG	UNP P00491
C	-12	ARG	-	EXPRESSION TAG	UNP P00491
C	-11	GLN	-	EXPRESSION TAG	UNP P00491
C	-10	HIS	-	EXPRESSION TAG	UNP P00491
C	-9	MET	-	EXPRESSION TAG	UNP P00491
C	-8	ASP	-	EXPRESSION TAG	UNP P00491
C	-7	SER	-	EXPRESSION TAG	UNP P00491
C	-6	GLY	-	EXPRESSION TAG	UNP P00491
C	-5	GLY	-	EXPRESSION TAG	UNP P00491

Continued on next page...

Continued from previous page...

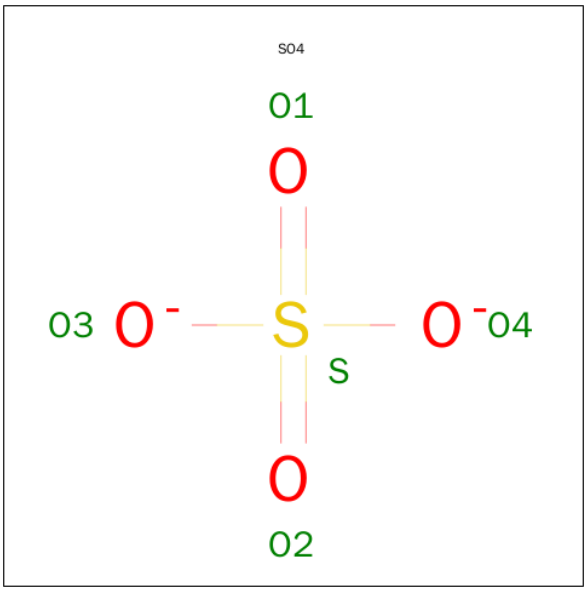
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	EXPRESSION TAG	UNP P00491
C	-3	GLY	-	EXPRESSION TAG	UNP P00491
C	-2	SER	-	EXPRESSION TAG	UNP P00491
C	-1	GLY	-	EXPRESSION TAG	UNP P00491
C	0	HIS	-	EXPRESSION TAG	UNP P00491
C	201	GLN	GLU	ENGINEERED	UNP P00491
C	243	ASP	ASN	ENGINEERED	UNP P00491

- Molecule 2 is 5-(6-AMINO-2-FLUORO-PURIN-9-YL)-2-HYDROXYMETHYL-TETRAHYDRO-FURAN-3-OL (three-letter code: 2FD) (formula: $C_{10}H_{12}FN_5O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			19	10	1	5	3		
2	B	1	Total	C	F	N	O	0	0
			19	10	1	5	3		
2	C	1	Total	C	F	N	O	0	0
			19	10	1	5	3		
2	C	1	Total	C	F	N	O	0	0
			19	10	1	5	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

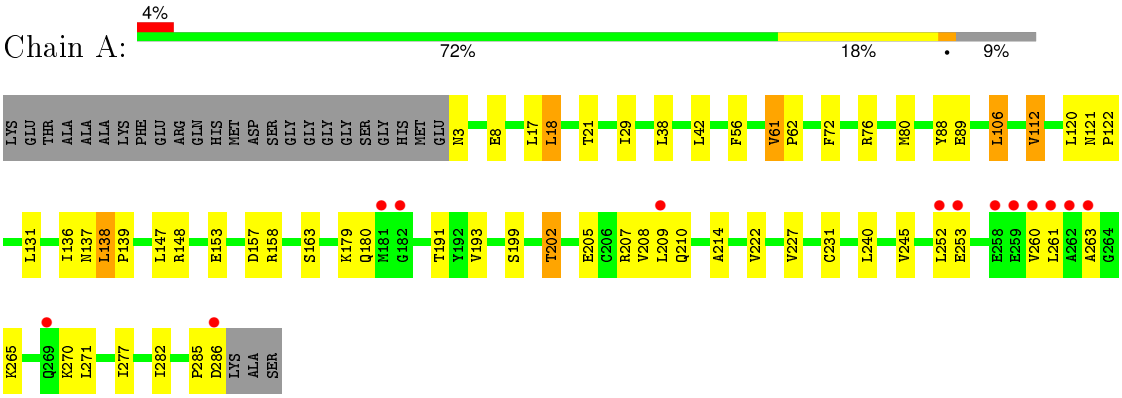
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	19	Total O 19 19	0	0
4	C	20	Total O 20 20	0	0

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.

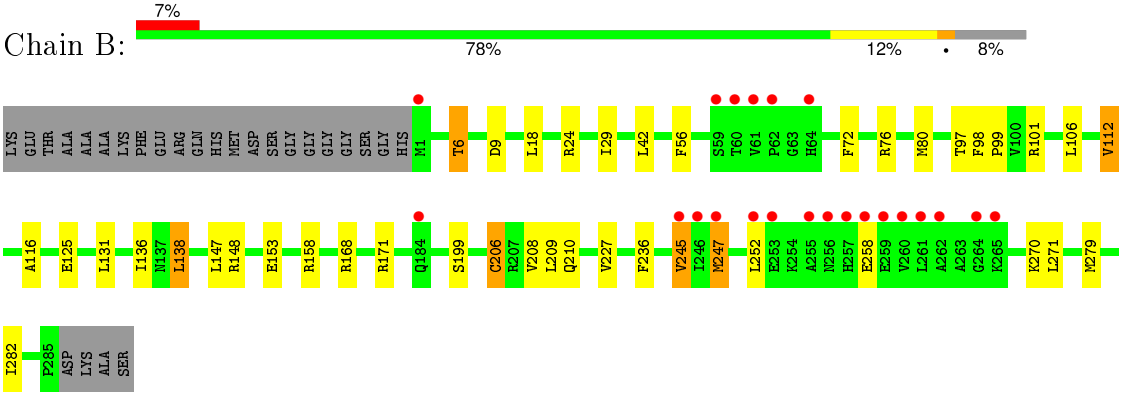
- Molecule 1: Purine nucleoside phosphorylase

Chain A:



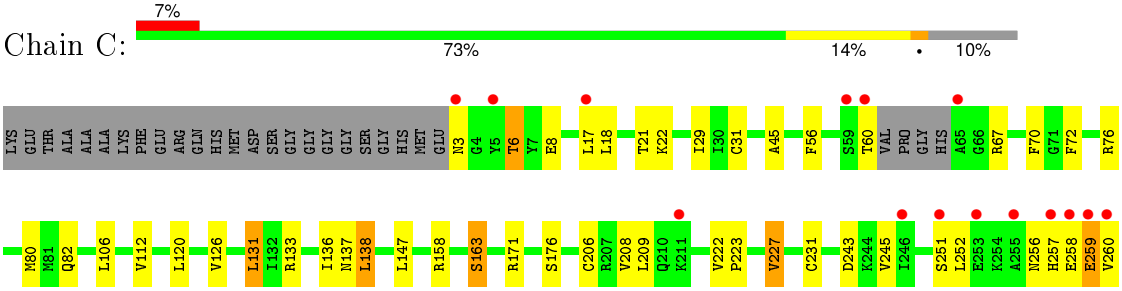
- Molecule 1: Purine nucleoside phosphorylase

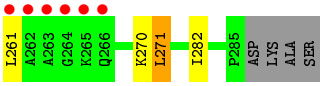
Chain B:



- Molecule 1: Purine nucleoside phosphorylase

Chain C:




L261
A262
A263
G264
K265
Q266
K270
L271
I282
P285
ASP
LYS
ALA
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.24Å 130.65Å 149.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.52 98.36 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.52) 98.7 (98.36-2.52)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.16 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0061	Depositor
R, R_{free}	0.212 , 0.251 0.220 , 0.260	Depositor DCC
R_{free} test set	2390 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 47485 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6904	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: SO4, 2FD

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	0.52	1/2262 (0.0%)	0.65	0/3062
1	B	0.43	0/2271	0.62	0/3073
1	C	0.45	1/2232 (0.0%)	0.62	0/3018
All	All	0.46	2/6765 (0.0%)	0.63	0/9153

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	CYS	CB-SG	-6.38	1.71	1.82
1	C	231	CYS	CB-SG	-5.26	1.73	1.81

There are no bond angle outliers.

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	2211	0	2183	31	0
1	B	2220	0	2197	23	0
1	C	2183	0	2161	20	0
2	A	19	0	12	0	0
2	B	19	0	12	1	0
2	C	38	0	24	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	50	0	0	1	0
3	B	50	0	0	0	0
3	C	50	0	0	0	0
4	A	25	0	0	1	0
4	B	19	0	0	1	0
4	C	20	0	0	0	0
All	All	6904	0	6589	73	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 (73) 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:120:LEU:HD23	1:A:245:VAL:HG21	1.67	0.77
1:A:163:SER:O	1:B:252:LEU:HD21	1.86	0.74
1:C:17:LEU:O	1:C:21:THR:HG22	1.89	0.72
1:C:76:ARG:NH2	1:C:282:ILE:O	2.23	0.72
1:A:29:ILE:HD12	1:A:80:MET:HE2	1.74	0.70
1:C:120:LEU:HD23	1:C:245:VAL:HG21	1.77	0.65
1:A:202:THR:HG23	1:A:205:GLU:OE1	1.97	0.65
1:B:6:THR:HG23	1:B:9:ASP:H	1.65	0.61
1:B:116:ALA:HB3	2:B:300:2FD:O3'	2.01	0.61
1:C:29:ILE:HD12	1:C:80:MET:CE	2.32	0.60
1:A:61:VAL:HG21	1:A:89:GLU:OE1	2.02	0.59
1:A:29:ILE:HG23	1:A:112:VAL:HG22	1.84	0.58
1:B:76:ARG:HG3	1:B:279:MET:HB3	1.86	0.58
1:B:29:ILE:HG12	1:B:112:VAL:HG13	1.86	0.57
1:C:258:GLU:O	1:C:259:GLU:HB2	2.03	0.57
1:C:126:VAL:HG22	1:C:243:ASP:HA	1.88	0.54
1:A:76:ARG:NH2	1:A:282:ILE:O	2.41	0.53
1:A:18:LEU:HD13	1:A:106:LEU:HD12	1.90	0.53
1:A:29:ILE:HD12	1:A:80:MET:CE	2.39	0.52
1:A:193:VAL:HB	1:A:214:ALA:CB	2.40	0.52
2:C:300:2FD:H2'1	2:C:300:2FD:N3	2.25	0.52
1:B:29:ILE:HD12	1:B:80:MET:HE2	1.92	0.51
1:C:29:ILE:HD12	1:C:80:MET:HE1	1.92	0.51
1:A:240:LEU:CD2	1:A:263:ALA:HB1	2.41	0.51
1:B:136:ILE:HG22	1:B:138:LEU:HD13	1.92	0.50
1:B:206:CYS:SG	1:B:245:VAL:HG23	2.51	0.50
1:C:29:ILE:HD12	1:C:80:MET:HE2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:O	1:A:286:ASP:C	2.51	0.48
1:A:136:ILE:HG13	1:A:191:THR:HG21	1.94	0.48
1:A:240:LEU:HD23	1:A:263:ALA:CB	2.43	0.48
1:B:112:VAL:HA	1:B:236:PHE:O	2.13	0.48
1:C:72:PHE:CE1	2:C:301:2FD:H2'1	2.49	0.48
1:A:207:ARG:HA	1:A:210:GLN:HE21	1.79	0.48
1:C:6:THR:HG23	1:C:8:GLU:H	1.79	0.47
1:A:157:ASP:HB3	4:A:329:HOH:O	2.14	0.47
1:B:210:GLN:HE22	1:B:247:MET:CB	2.27	0.47
1:B:6:THR:HG23	1:B:9:ASP:N	2.30	0.47
1:B:101:ARG:NE	4:B:308:HOH:O	2.47	0.47
1:A:61:VAL:HG13	1:A:62:PRO:HD2	1.97	0.47
1:A:138:LEU:O	1:A:139:PRO:C	2.52	0.47
1:B:72:PHE:HA	1:B:76:ARG:O	2.15	0.47
1:A:42:LEU:HD21	1:A:80:MET:HE1	1.96	0.47
1:A:72:PHE:HA	1:A:76:ARG:O	2.14	0.46
1:B:210:GLN:HE22	1:B:247:MET:HB3	1.79	0.46
1:A:193:VAL:HB	1:A:214:ALA:HB2	1.98	0.46
1:C:223:PRO:O	1:C:227:VAL:HG13	2.15	0.45
1:C:258:GLU:OE1	1:C:260:VAL:HG13	2.16	0.45
1:B:42:LEU:HD21	1:B:80:MET:HE1	1.98	0.45
1:A:240:LEU:HD23	1:A:263:ALA:HB2	1.99	0.45
1:B:6:THR:HG22	1:B:9:ASP:OD2	2.17	0.44
1:A:137:ASN:HB2	1:A:222:VAL:HG11	1.99	0.44
1:A:252:LEU:HD11	1:C:163:SER:HB2	1.99	0.44
1:C:45:ALA:HA	1:C:70:PHE:O	2.17	0.43
1:C:137:ASN:HB2	1:C:222:VAL:HG11	2.00	0.43
1:A:240:LEU:HD21	1:A:263:ALA:HB1	2.01	0.43
1:C:206:CYS:SG	1:C:245:VAL:HG23	2.59	0.43
1:C:136:ILE:HG22	1:C:138:LEU:HD13	1.99	0.43
1:A:29:ILE:HG23	1:A:112:VAL:CG2	2.46	0.43
1:B:97:THR:HB	1:B:227:VAL:HG11	2.00	0.42
1:A:17:LEU:O	1:A:21:THR:HG22	2.19	0.42
1:A:120:LEU:HD23	1:A:245:VAL:CG2	2.45	0.42
1:B:206:CYS:SG	1:B:245:VAL:CG2	3.08	0.42
1:A:121:ASN:O	1:A:122:PRO:C	2.56	0.42
1:B:42:LEU:HD21	1:B:80:MET:CE	2.50	0.41
1:C:271:LEU:HD22	1:C:271:LEU:O	2.20	0.41
1:A:265:LYS:N	3:A:298:SO4:O4	2.53	0.41
1:B:98:PHE:HB3	1:B:99:PRO:HD3	2.03	0.41
1:A:88:TYR:CE2	1:A:89:GLU:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LEU:HD11	1:C:171:ARG:HA	2.04	0.40
1:B:29:ILE:HG23	1:B:112:VAL:HG22	2.03	0.40
1:B:168:ARG:HA	1:B:171:ARG:NH1	2.36	0.40
1:C:67:ARG:HE	1:C:82:GLN:NE2	2.19	0.40
1:B:76:ARG:NH2	1:B:282:ILE:O	2.54	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	282/311 (91%)	270 (96%)	11 (4%)	1 (0%)	39 60
1	B	283/311 (91%)	271 (96%)	12 (4%)	0	100 100
1	C	275/311 (88%)	266 (97%)	6 (2%)	3 (1%)	17 30
All	All	840/933 (90%)	807 (96%)	29 (4%)	4 (0%)	34 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	259	GLU
1	C	257	HIS
1	A	260	VAL
1	C	261	LEU

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	233/253 (92%)	207 (89%)	26 (11%)	7 13
1	B	234/253 (92%)	212 (91%)	22 (9%)	11 19
1	C	231/253 (91%)	207 (90%)	24 (10%)	9 15
All	All	698/759 (92%)	626 (90%)	72 (10%)	9 16

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	8	GLU
1	A	18	LEU
1	A	38	LEU
1	A	56	PHE
1	A	61	VAL
1	A	106	LEU
1	A	112	VAL
1	A	131	LEU
1	A	138	LEU
1	A	147	LEU
1	A	148	ARG
1	A	153	GLU
1	A	158	ARG
1	A	179	LYS
1	A	180	GLN
1	A	199	SER
1	A	202	THR
1	A	208	VAL
1	A	209	LEU
1	A	227	VAL
1	A	253	GLU
1	A	261	LEU
1	A	270	LYS
1	A	271	LEU
1	A	277	ILE
1	B	6	THR
1	B	18	LEU
1	B	24	ARG
1	B	56	PHE
1	B	106	LEU
1	B	112	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	125	GLU
1	B	131	LEU
1	B	138	LEU
1	B	147	LEU
1	B	148	ARG
1	B	153	GLU
1	B	158	ARG
1	B	199	SER
1	B	206	CYS
1	B	208	VAL
1	B	209	LEU
1	B	245	VAL
1	B	247	MET
1	B	258	GLU
1	B	270	LYS
1	B	271	LEU
1	C	3	ASN
1	C	6	THR
1	C	18	LEU
1	C	22	LYS
1	C	31	CYS
1	C	56	PHE
1	C	60	THR
1	C	106	LEU
1	C	112	VAL
1	C	131	LEU
1	C	133	ARG
1	C	138	LEU
1	C	147	LEU
1	C	158	ARG
1	C	163	SER
1	C	176	SER
1	C	208	VAL
1	C	209	LEU
1	C	227	VAL
1	C	251	SER
1	C	252	LEU
1	C	256	ASN
1	C	270	LYS
1	C	271	LEU

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

Mol	Chain	Res	Type
1	A	3	ASN
1	A	180	GLN
1	A	210	GLN
1	A	269	GLN
1	B	172	GLN
1	B	180	GLN
1	B	210	GLN
1	C	55	ASN
1	C	82	GLN
1	C	256	ASN
1	C	266	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

34 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	SO4	A	290	-	4,4,4	0.49	0	6,6,6	0.38	0
3	SO4	A	291	-	4,4,4	0.27	0	6,6,6	0.24	0
3	SO4	A	292	-	4,4,4	0.36	0	6,6,6	0.25	0
3	SO4	A	293	-	4,4,4	0.11	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	A	294	-	4,4,4	0.17	0	6,6,6	0.23	0
3	SO4	A	295	-	4,4,4	0.08	0	6,6,6	0.35	0
3	SO4	A	296	-	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	A	297	-	4,4,4	0.13	0	6,6,6	0.16	0
3	SO4	A	298	-	4,4,4	0.20	0	6,6,6	0.12	0
3	SO4	A	299	-	4,4,4	0.17	0	6,6,6	0.25	0
2	2FD	A	300	-	17,21,21	1.73	2 (11%)	20,31,31	2.73	4 (20%)
3	SO4	B	290	-	4,4,4	0.35	0	6,6,6	0.41	0
3	SO4	B	291	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	B	292	-	4,4,4	0.21	0	6,6,6	0.31	0
3	SO4	B	293	-	4,4,4	0.16	0	6,6,6	0.31	0
3	SO4	B	294	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	B	295	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SO4	B	296	-	4,4,4	0.12	0	6,6,6	0.26	0
3	SO4	B	297	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	B	298	-	4,4,4	0.22	0	6,6,6	0.22	0
3	SO4	B	299	-	4,4,4	0.19	0	6,6,6	0.11	0
2	2FD	B	300	-	17,21,21	1.62	2 (11%)	20,31,31	2.67	6 (30%)
3	SO4	C	290	-	4,4,4	0.61	0	6,6,6	0.32	0
3	SO4	C	291	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	C	292	-	4,4,4	0.21	0	6,6,6	0.12	0
3	SO4	C	293	-	4,4,4	0.23	0	6,6,6	0.22	0
3	SO4	C	294	-	4,4,4	0.16	0	6,6,6	0.23	0
3	SO4	C	295	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	C	296	-	4,4,4	0.27	0	6,6,6	0.13	0
3	SO4	C	297	-	4,4,4	0.19	0	6,6,6	0.20	0
3	SO4	C	298	-	4,4,4	0.20	0	6,6,6	0.07	0
3	SO4	C	299	-	4,4,4	0.17	0	6,6,6	0.13	0
2	2FD	C	300	-	17,21,21	1.43	2 (11%)	20,31,31	2.92	4 (20%)
2	2FD	C	301	-	17,21,21	1.83	2 (11%)	20,31,31	2.91	8 (40%)

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	SO4	A	290	-	-	0/0/0/0	0/0/0/0
3	SO4	A	291	-	-	0/0/0/0	0/0/0/0
3	SO4	A	292	-	-	0/0/0/0	0/0/0/0
3	SO4	A	293	-	-	0/0/0/0	0/0/0/0
3	SO4	A	294	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	295	-	-	0/0/0/0	0/0/0/0
3	SO4	A	296	-	-	0/0/0/0	0/0/0/0
3	SO4	A	297	-	-	0/0/0/0	0/0/0/0
3	SO4	A	298	-	-	0/0/0/0	0/0/0/0
3	SO4	A	299	-	-	0/0/0/0	0/0/0/0
2	2FD	A	300	-	-	0/2/18/18	0/3/3/3
3	SO4	B	290	-	-	0/0/0/0	0/0/0/0
3	SO4	B	291	-	-	0/0/0/0	0/0/0/0
3	SO4	B	292	-	-	0/0/0/0	0/0/0/0
3	SO4	B	293	-	-	0/0/0/0	0/0/0/0
3	SO4	B	294	-	-	0/0/0/0	0/0/0/0
3	SO4	B	295	-	-	0/0/0/0	0/0/0/0
3	SO4	B	296	-	-	0/0/0/0	0/0/0/0
3	SO4	B	297	-	-	0/0/0/0	0/0/0/0
3	SO4	B	298	-	-	0/0/0/0	0/0/0/0
3	SO4	B	299	-	-	0/0/0/0	0/0/0/0
2	2FD	B	300	-	-	0/2/18/18	0/3/3/3
3	SO4	C	290	-	-	0/0/0/0	0/0/0/0
3	SO4	C	291	-	-	0/0/0/0	0/0/0/0
3	SO4	C	292	-	-	0/0/0/0	0/0/0/0
3	SO4	C	293	-	-	0/0/0/0	0/0/0/0
3	SO4	C	294	-	-	0/0/0/0	0/0/0/0
3	SO4	C	295	-	-	0/0/0/0	0/0/0/0
3	SO4	C	296	-	-	0/0/0/0	0/0/0/0
3	SO4	C	297	-	-	0/0/0/0	0/0/0/0
3	SO4	C	298	-	-	0/0/0/0	0/0/0/0
3	SO4	C	299	-	-	0/0/0/0	0/0/0/0
2	2FD	C	300	-	-	0/2/18/18	0/3/3/3
2	2FD	C	301	-	-	0/2/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	2FD	C2-N3	2.82	1.34	1.31
2	B	300	2FD	C2-N3	4.13	1.35	1.31
2	C	300	2FD	C2-N1	4.61	1.36	1.31
2	A	300	2FD	C2-N1	4.68	1.36	1.31
2	B	300	2FD	C2-N1	4.75	1.36	1.31
2	A	300	2FD	C2-N3	4.79	1.36	1.31
2	C	301	2FD	C2-N3	4.80	1.36	1.31
2	C	301	2FD	C2-N1	5.41	1.36	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	2FD	N3-C2-N1	-7.53	121.16	131.11
2	C	301	2FD	N3-C2-N1	-7.44	121.28	131.11
2	C	300	2FD	N3-C2-N1	-7.37	121.38	131.11
2	B	300	2FD	N3-C2-N1	-7.33	121.43	131.11
2	C	300	2FD	C4-C5-N7	-3.05	106.67	109.48
2	C	301	2FD	C4-C5-N7	-3.04	106.69	109.48
2	C	301	2FD	C2-N1-C6	2.05	120.42	115.03
2	B	300	2FD	C2-N1-C6	2.07	120.47	115.03
2	C	301	2FD	C3'-C2'-C1'	2.16	107.60	102.40
2	B	300	2FD	O4'-C1'-N9	2.92	112.77	107.72
2	B	300	2FD	C2-N3-C4	3.52	119.86	114.93
2	A	300	2FD	C2-N3-C4	3.84	120.30	114.93
2	C	301	2FD	O4'-C1'-N9	3.91	114.48	107.72
2	C	301	2FD	C2-N3-C4	4.04	120.59	114.93
2	A	300	2FD	F-C2-N3	4.17	118.41	114.44
2	B	300	2FD	F-C2-N3	4.17	118.42	114.44
2	C	301	2FD	F-C2-N3	4.29	118.53	114.44
2	C	300	2FD	C2-N3-C4	4.34	121.01	114.93
2	B	300	2FD	F-C2-N1	5.99	120.15	114.44
2	C	301	2FD	F-C2-N1	6.04	120.19	114.44
2	A	300	2FD	F-C2-N1	6.28	120.43	114.44
2	C	300	2FD	F-C2-N1	8.26	122.31	114.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	298	SO4	1	0
2	B	300	2FD	1	0
2	C	300	2FD	1	0
2	C	301	2FD	1	0

5.7 Other polymers (i)

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	284/311 (91%)	0.71	13 (4%)	36	42	26, 47, 76, 88	0
1	B	285/311 (91%)	0.73	22 (7%)	16	18	28, 47, 84, 108	0
1	C	279/311 (89%)	0.83	21 (7%)	17	19	29, 47, 76, 95	0
All	All	848/933 (90%)	0.76	56 (6%)	22	24	26, 47, 79, 108	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	261	LEU	16.9
1	C	260	VAL	15.5
1	B	261	LEU	8.3
1	C	257	HIS	7.1
1	C	258	GLU	6.5
1	B	64	HIS	6.1
1	B	256	ASN	5.8
1	C	59	SER	5.7
1	A	182	GLY	5.6
1	B	252	LEU	5.4
1	B	61	VAL	5.4
1	B	255	ALA	4.9
1	C	60	THR	4.5
1	A	261	LEU	4.4
1	A	258	GLU	4.2
1	B	257	HIS	4.2
1	B	253	GLU	4.2
1	C	264	GLY	4.1
1	C	251	SER	4.0
1	A	262	ALA	4.0
1	B	62	PRO	4.0
1	A	181	MET	3.9
1	A	259	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	253	GLU	3.8
1	C	259	GLU	3.8
1	B	60	THR	3.7
1	B	260	VAL	3.6
1	B	258	GLU	3.6
1	A	286	ASP	3.6
1	B	246	ILE	3.4
1	B	259	GLU	3.4
1	A	260	VAL	3.0
1	B	59	SER	2.9
1	C	246	ILE	2.9
1	C	3	ASN	2.9
1	B	247	MET	2.8
1	A	252	LEU	2.6
1	C	65	ALA	2.6
1	B	265	LYS	2.5
1	C	262	ALA	2.5
1	B	262	ALA	2.4
1	C	255	ALA	2.4
1	B	1	MET	2.3
1	C	253	GLU	2.3
1	A	263	ALA	2.3
1	B	245	VAL	2.3
1	C	266	GLN	2.2
1	B	184	GLN	2.2
1	C	211	LYS	2.2
1	C	263	ALA	2.2
1	B	264	GLY	2.2
1	C	265	LYS	2.1
1	C	17	LEU	2.1
1	A	269	GLN	2.1
1	A	209	LEU	2.0
1	C	5	TYR	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	SO4	C	294	5/5	0.83	0.26	3.30	83,84,85,85	0
2	2FD	C	301	19/19	0.77	0.30	3.04	82,85,90,91	0
3	SO4	C	296	5/5	0.83	0.35	1.14	131,131,132,132	0
2	2FD	A	300	19/19	0.90	0.20	-0.14	58,63,70,71	0
2	2FD	B	300	19/19	0.90	0.19	-0.29	62,65,69,70	0
3	SO4	B	296	5/5	0.91	0.18	-0.31	92,92,93,93	0
2	2FD	C	300	19/19	0.90	0.18	-0.33	72,75,82,83	0
3	SO4	B	292	5/5	0.96	0.13	-0.57	63,63,66,67	0
3	SO4	C	290	5/5	0.98	0.14	-0.88	45,46,48,50	0
3	SO4	A	296	5/5	0.96	0.17	-0.92	88,88,89,89	0
3	SO4	B	294	5/5	0.92	0.14	-1.15	96,97,97,98	0
3	SO4	A	295	5/5	0.89	0.16	-1.17	76,77,77,78	0
3	SO4	A	290	5/5	0.98	0.15	-1.25	44,44,46,46	0
3	SO4	B	290	5/5	0.99	0.13	-1.44	38,42,42,43	0
3	SO4	C	292	5/5	0.97	0.10	-1.94	70,70,70,72	0
3	SO4	A	292	5/5	0.99	0.11	-2.15	46,47,49,50	0
3	SO4	A	293	5/5	0.92	0.12	-2.24	66,67,69,69	0
3	SO4	C	291	5/5	0.98	0.11	-2.51	54,55,57,58	0
3	SO4	A	291	5/5	0.98	0.12	-2.71	49,50,51,51	0
3	SO4	C	297	5/5	0.91	0.20	-	108,108,109,109	0
3	SO4	A	297	5/5	0.85	0.15	-	89,89,90,91	0
3	SO4	B	297	5/5	0.94	0.15	-	99,99,99,100	0
3	SO4	B	293	5/5	0.90	0.25	-	88,89,89,89	0
3	SO4	C	295	5/5	0.92	0.14	-	94,94,95,95	0
3	SO4	C	298	5/5	0.81	0.26	-	118,118,118,119	0
3	SO4	B	295	5/5	0.64	0.24	-	111,111,112,112	0
3	SO4	C	299	5/5	0.92	0.38	-	102,102,102,103	0
3	SO4	B	291	5/5	0.94	0.17	-	76,76,77,77	0
3	SO4	A	294	5/5	0.95	0.23	-	85,85,86,86	0
3	SO4	B	298	5/5	0.78	0.18	-	116,116,117,117	0
3	SO4	A	299	5/5	0.87	0.18	-	98,99,99,100	0
3	SO4	C	293	5/5	0.94	0.17	-	81,81,81,82	0
3	SO4	B	299	5/5	0.91	0.22	-	100,101,101,101	0
3	SO4	A	298	5/5	0.84	0.18	-	103,104,104,104	0

6.5 Other polymers (i)

There are no such residues in this entry.