Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:03 PM GMT

PDB ID	:	1N8F
Title	:	Crystal structure of E24Q mutant of phenylalanine-regulated 3-deoxy-D-ara bino-heptulosonate-7-phosphate synthase (DAHP synthase) from Escherichia Coli in complex with Mn2+ and PEP
Authors	:	Shumilin, I.A.; Bauerle, R.; Kretsinger, R.H.
Deposited on	:	2002-11-20
Resolution	:	1.75 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:

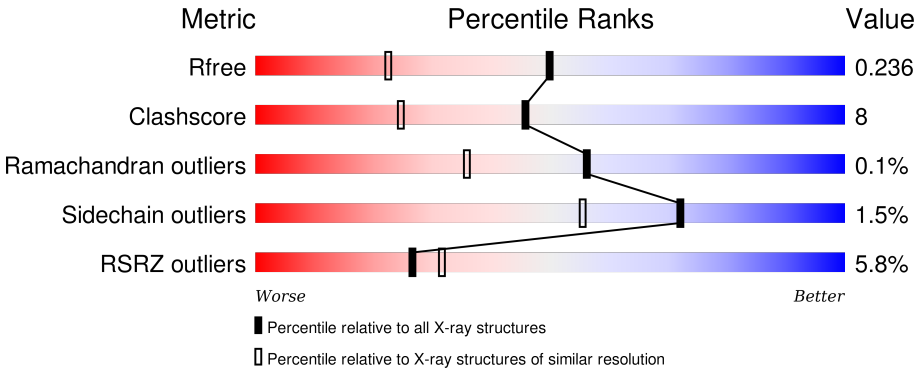
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	350	5% 83% 14%
1	B	350	% 89% 9%
1	C	350	8% 77% 19%
1	D	350	8% 83% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	5353	-	-	-	X
3	SO4	B	2353	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11934 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 DAHP Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	3	0
			2621	1646	466	495	14			
1	B	343	Total	C	N	O	S	0	3	0
			2618	1644	465	495	14			
1	C	343	Total	C	N	O	S	0	0	0
			2606	1637	465	490	14			
1	D	343	Total	C	N	O	S	0	1	0
			2610	1639	465	492	14			

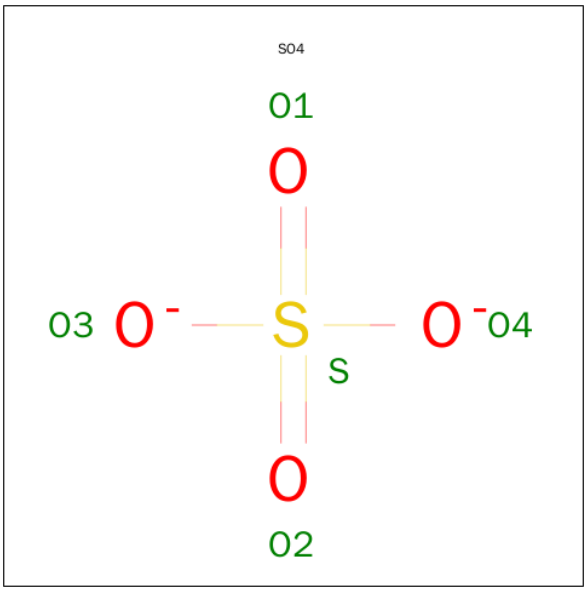
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLN	GLU	ENGINEERED	UNP P0AB91
B	24	GLN	GLU	ENGINEERED	UNP P0AB91
C	24	GLN	GLU	ENGINEERED	UNP P0AB91
D	24	GLN	GLU	ENGINEERED	UNP P0AB91

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

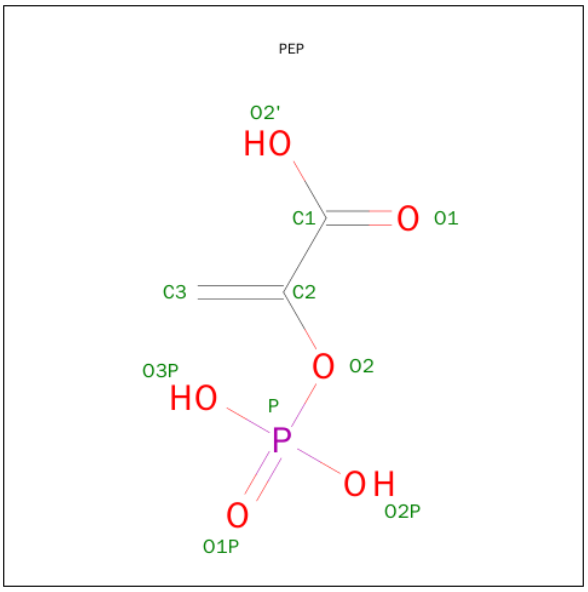
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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



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

- Molecule 4 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 10 3 6 1	0	0
4	B	1	Total C O P 10 3 6 1	0	0
4	C	1	Total C O P 10 3 6 1	0	0
4	D	1	Total C O P 10 3 6 1	0	0

- Molecule 5 is water.

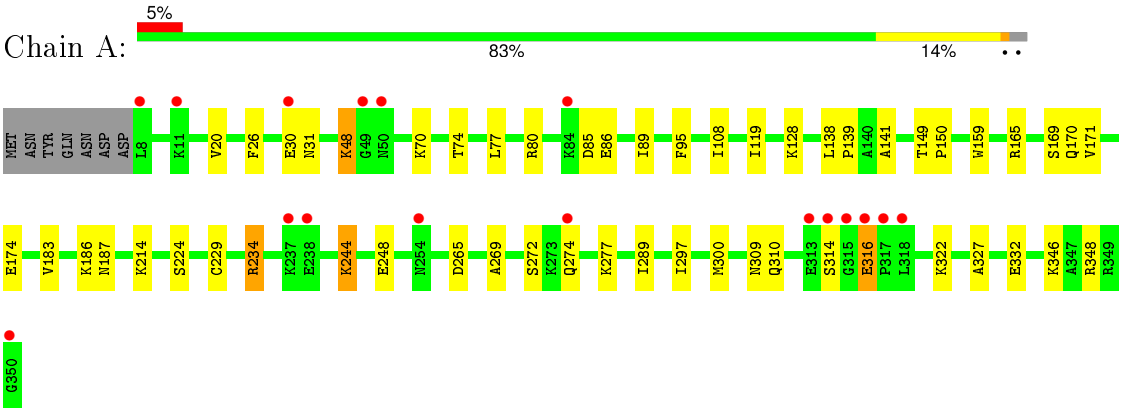
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	369	Total O 369 369	0	0
5	B	394	Total O 394 394	0	0
5	C	318	Total O 318 318	0	0
5	D	314	Total O 314 314	0	0

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.

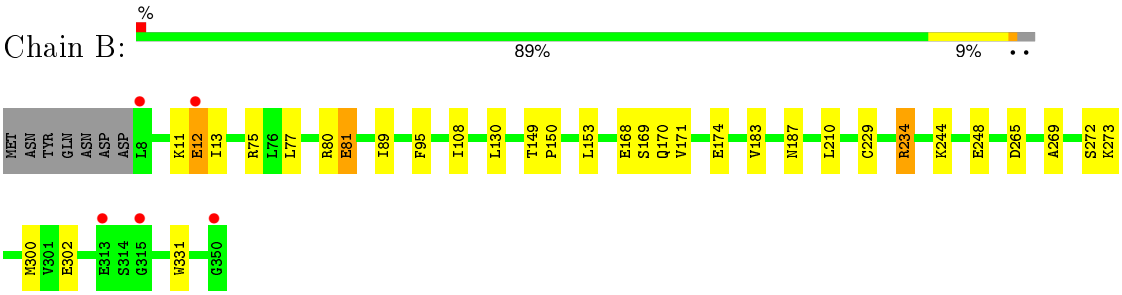
- Molecule 1: DAHP Synthetase

Chain A:



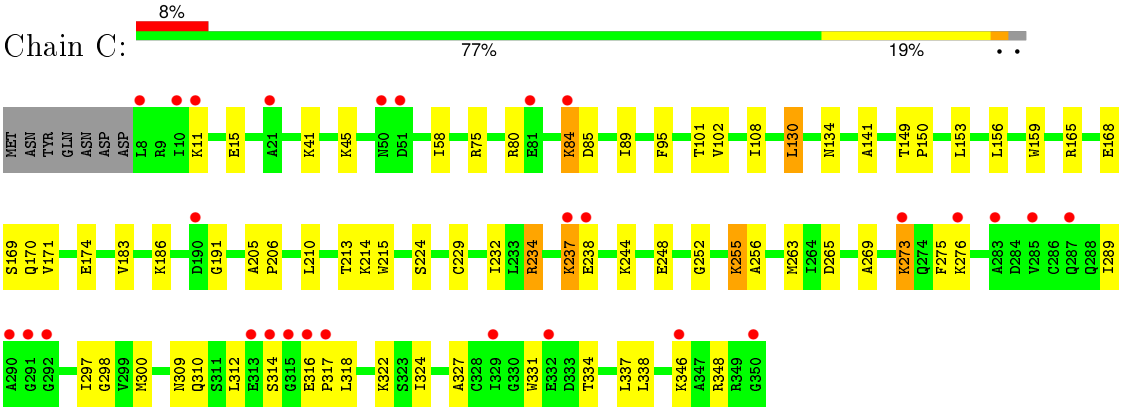
- Molecule 1: DAHP Synthetase

Chain B:



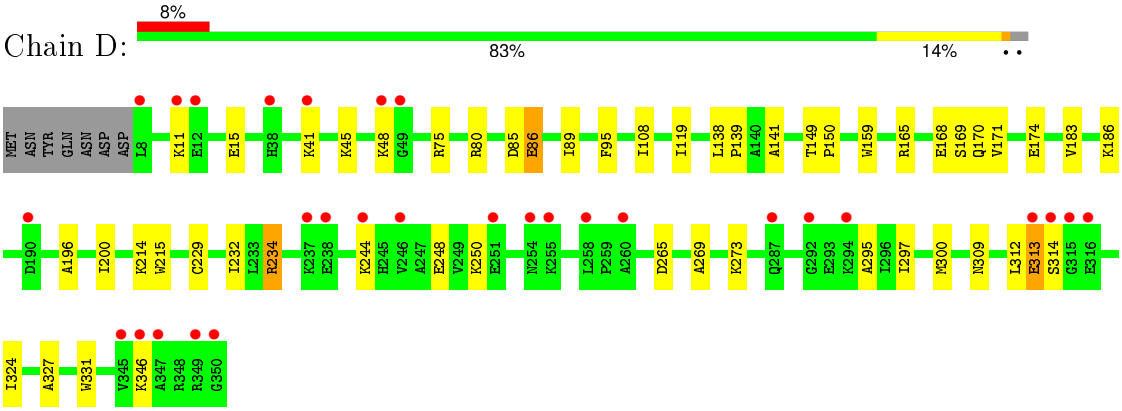
- Molecule 1: DAHP Synthetase

Chain C:



• Molecule 1: DAHP Synthetase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	213.22Å 53.28Å 150.25Å 90.00° 116.90° 90.00°	Depositor
Resolution (Å)	20.00 – 1.75 18.80 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-1.75) 99.4 (18.80-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.75Å)	Xtriage
Refinement program	CNS, ARP	Depositor
R, R_{free}	0.209 , 0.237 0.208 , 0.236	Depositor DCC
R_{free} test set	3033 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 151346 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11934	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: MN, PEP, 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	0.33	0/2678	0.57	0/3620
1	B	0.38	2/2675 (0.1%)	0.63	4/3616 (0.1%)
1	C	0.26	0/2651	0.52	0/3584
1	D	0.28	0/2659	0.55	0/3595
All	All	0.32	2/10663 (0.0%)	0.57	4/14415 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81[A]	GLU	CB-CG	5.15	1.61	1.52
1	B	81[B]	GLU	CB-CG	5.15	1.61	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	12[A]	GLU	N-CA-CB	5.75	120.95	110.60
1	B	12[B]	GLU	N-CA-CB	5.75	120.95	110.60
1	B	81[A]	GLU	N-CA-CB	-5.34	100.99	110.60
1	B	81[B]	GLU	N-CA-CB	-5.34	100.99	110.60

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	2621	0	2645	38	0
1	B	2618	0	2642	24	0
1	C	2606	0	2637	72	0
1	D	2610	0	2637	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	10	0	2	1	0
4	B	10	0	2	0	0
4	C	10	0	2	0	0
4	D	10	0	2	0	0
5	A	369	0	0	5	0
5	B	394	0	0	2	0
5	C	318	0	0	5	0
5	D	314	0	0	4	0
All	All	11934	0	10569	162	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 8.

All (162) 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:C:101:THR:HG23	1:C:102:VAL:H	1.20	1.05
1:C:213:THR:HG23	1:C:215:TRP:H	1.41	0.85
1:A:30[B]:GLU:HG3	1:A:31:ASN:N	1.91	0.85
1:C:130:LEU:HD12	1:C:156:LEU:HB3	1.60	0.82
1:C:80:ARG:HA	1:C:89:ILE:HD12	1.62	0.81
1:B:77:LEU:O	1:B:81[A]:GLU:HG3	1.86	0.76
1:C:334:THR:O	1:C:338:LEU:HD13	1.85	0.75
1:C:314:SER:HB2	1:C:316:GLU:OE2	1.87	0.75
1:D:48:LYS:HA	1:D:48:LYS:HE2	1.69	0.74
1:A:244:LYS:H	1:A:244:LYS:HE3	1.53	0.74
1:C:101:THR:HG23	1:C:102:VAL:N	1.98	0.74
1:C:237:LYS:HE2	1:C:237:LYS:N	2.06	0.71
1:C:234:ARG:O	1:C:269:ALA:HB3	1.92	0.69
1:C:101:THR:CG2	1:C:102:VAL:H	2.03	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:HA	1:A:89:ILE:HD12	1.73	0.69
1:C:186:LYS:HD3	1:C:234:ARG:HG2	1.76	0.67
1:A:48:LYS:HA	1:A:48:LYS:HE3	1.75	0.66
1:A:272:SER:O	1:A:274[B]:GLN:HG2	1.96	0.66
1:B:272:SER:C	1:B:273:LYS:HD2	2.17	0.65
1:C:11:LYS:HE2	1:C:11:LYS:HA	1.78	0.65
1:A:169:SER:OG	1:A:171:VAL:HG22	1.96	0.65
1:B:273:LYS:N	1:B:273:LYS:HD2	2.11	0.65
1:D:169:SER:OG	1:D:171:VAL:HG22	1.98	0.63
1:B:300:MET:HG2	5:B:2580:HOH:O	1.98	0.62
1:C:273:LYS:HD2	1:C:273:LYS:O	2.00	0.62
1:D:312:LEU:HD11	1:D:324:ILE:HD12	1.82	0.61
1:C:169:SER:OG	1:C:171:VAL:HG22	2.00	0.61
1:B:130:LEU:HD12	1:B:153:LEU:HD22	1.83	0.61
1:D:80:ARG:HA	1:D:89:ILE:HD12	1.82	0.60
1:D:170:GLN:O	1:D:174:GLU:HG3	2.02	0.60
1:A:74:THR:HG22	5:A:5575:HOH:O	2.01	0.59
1:D:244:LYS:O	1:D:248:GLU:HG3	2.02	0.59
1:C:300:MET:HG2	5:C:3579:HOH:O	2.01	0.59
1:C:108:ILE:HD11	1:C:153:LEU:HD11	1.84	0.59
1:B:170:GLN:O	1:B:174:GLU:HG3	2.02	0.58
1:A:224:SER:HB3	1:B:11:LYS:HD3	1.85	0.58
1:C:237:LYS:HE2	1:C:237:LYS:H	1.67	0.56
1:A:95:PHE:HB3	1:A:108:ILE:HG13	1.87	0.56
1:C:310:GLN:NE2	1:C:322:LYS:HB3	2.21	0.56
1:D:300:MET:HG2	5:D:4575:HOH:O	2.05	0.55
1:C:95:PHE:HE1	1:C:130:LEU:HD23	1.72	0.55
1:A:170:GLN:O	1:A:174:GLU:HG3	2.07	0.55
1:C:58:ILE:HD13	1:C:338:LEU:HD11	1.89	0.54
1:A:244:LYS:H	1:A:244:LYS:CE	2.19	0.54
1:A:274[A]:GLN:HG3	5:A:5543:HOH:O	2.06	0.54
1:C:224:SER:HA	1:D:11:LYS:HE3	1.90	0.54
1:B:169:SER:OG	1:B:171:VAL:HG22	2.08	0.53
1:D:85[B]:ASP:HB2	1:D:86:GLU:OE1	2.09	0.53
1:D:234:ARG:O	1:D:269:ALA:HB3	2.08	0.53
1:A:314:SER:HB2	1:A:316:GLU:OE2	2.09	0.52
1:C:289:ILE:HG23	1:C:348:ARG:HD3	1.93	0.51
1:D:149:THR:N	1:D:150:PRO:CD	2.74	0.51
1:A:141:ALA:HB1	1:A:159:TRP:HE3	1.74	0.51
1:C:213:THR:HG23	1:C:215:TRP:N	2.18	0.51
1:C:252:GLY:O	1:C:255:LYS:HE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLU:HG2	1:D:165:ARG:HB3	1.92	0.51
1:C:149:THR:N	1:C:150:PRO:CD	2.74	0.51
1:D:273:LYS:NZ	1:D:273:LYS:HB3	2.26	0.51
1:D:86:GLU:HG2	1:D:346:LYS:HG3	1.93	0.50
1:D:312:LEU:O	1:D:314:SER:N	2.44	0.50
1:B:244:LYS:O	1:B:248:GLU:HG3	2.11	0.50
1:C:165:ARG:HB3	1:D:168:GLU:HG2	1.93	0.50
1:A:149:THR:N	1:A:150:PRO:CD	2.75	0.50
1:B:265:ASP:HA	1:B:300:MET:HB3	1.93	0.50
1:C:171:VAL:HG12	5:D:4441:HOH:O	2.10	0.50
1:C:191:GLY:HA3	1:C:237:LYS:NZ	2.27	0.50
1:A:86:GLU:HG2	1:A:346:LYS:HG3	1.93	0.50
1:C:41:LYS:HE2	1:C:45:LYS:NZ	2.27	0.50
1:D:196:ALA:O	1:D:200:ILE:HG13	2.12	0.50
1:A:234:ARG:O	1:A:269:ALA:HB3	2.12	0.50
1:A:265:ASP:HA	1:A:300:MET:HB3	1.95	0.49
1:C:265:ASP:HA	1:C:300:MET:HB3	1.94	0.49
1:A:310:GLN:NE2	1:A:322:LYS:HB3	2.27	0.49
1:B:80:ARG:HA	1:B:89:ILE:HD12	1.94	0.49
1:D:214:LYS:HE3	1:D:215:TRP:CZ2	2.47	0.49
1:A:289:ILE:O	1:A:348:ARG:HB2	2.11	0.49
1:A:165:ARG:HB3	1:B:168:GLU:HG2	1.95	0.49
1:D:15:GLU:HG2	5:D:4621:HOH:O	2.12	0.49
1:C:214:LYS:HE3	1:C:215:TRP:CZ2	2.48	0.49
1:A:169:SER:HG	1:A:171:VAL:HG22	1.77	0.49
1:C:169:SER:HG	1:C:171:VAL:HG22	1.78	0.49
1:B:11:LYS:NZ	1:B:11:LYS:HB3	2.27	0.49
1:C:237:LYS:HE2	1:C:238:GLU:H	1.78	0.48
1:C:11:LYS:HE2	1:C:11:LYS:CA	2.43	0.48
1:D:313:GLU:CD	1:D:313:GLU:H	2.17	0.48
1:D:265:ASP:HA	1:D:300:MET:HB3	1.96	0.48
1:D:250:LYS:HD3	1:D:295:ALA:CB	2.43	0.48
1:D:141:ALA:HB1	1:D:159:TRP:HE3	1.79	0.47
1:A:70:LYS:O	1:A:74:THR:HG23	2.14	0.47
1:D:214:LYS:HE3	1:D:215:TRP:CE2	2.49	0.47
1:B:11:LYS:HB2	1:B:12[B]:GLU:HG3	1.95	0.47
1:B:234:ARG:O	1:B:269:ALA:HB3	2.15	0.47
1:B:11:LYS:CB	1:B:12[B]:GLU:HG3	2.44	0.47
1:C:130:LEU:CD1	1:C:134:ASN:ND2	2.78	0.47
1:D:41:LYS:HZ3	1:D:45:LYS:HE3	1.80	0.47
1:A:244:LYS:O	1:A:248:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:LEU:C	1:D:314:SER:H	2.19	0.46
1:D:95:PHE:HB3	1:D:108:ILE:HG13	1.97	0.46
1:B:169:SER:HG	1:B:171:VAL:HG22	1.80	0.46
1:B:149:THR:N	1:B:150:PRO:CD	2.79	0.46
1:A:274[A]:GLN:HB3	1:A:277:LYS:CG	2.46	0.46
1:C:75:ARG:HB3	1:C:331:TRP:CZ2	2.51	0.46
1:C:80:ARG:CA	1:C:89:ILE:HD12	2.40	0.46
1:D:183:VAL:O	1:D:229:CYS:HA	2.16	0.45
1:C:324:ILE:HG12	5:C:3436:HOH:O	2.16	0.45
1:C:316:GLU:N	1:C:316:GLU:OE2	2.49	0.45
1:C:95:PHE:HB3	1:C:108:ILE:HG13	1.99	0.45
1:B:183:VAL:O	1:B:229:CYS:HA	2.16	0.45
1:C:95:PHE:CE1	1:C:130:LEU:HD23	2.51	0.45
1:C:237:LYS:HG2	1:C:238:GLU:HG2	1.98	0.45
1:A:119:ILE:HG21	1:B:210:LEU:HD21	1.98	0.45
1:C:252:GLY:O	1:C:255:LYS:HG3	2.16	0.45
1:B:95:PHE:HB3	1:B:108:ILE:HG13	1.99	0.45
1:D:186:LYS:HD3	1:D:234:ARG:HG2	1.98	0.44
1:C:130:LEU:CD1	1:C:134:ASN:HD22	2.31	0.44
1:C:275:PHE:CE1	1:C:276:LYS:HG3	2.53	0.44
1:C:170:GLN:O	1:C:174:GLU:HG3	2.18	0.44
1:C:84:LYS:C	1:C:84:LYS:HD3	2.39	0.44
1:A:85:ASP:HB2	5:A:5557:HOH:O	2.18	0.44
1:C:244:LYS:O	1:C:248:GLU:HG3	2.18	0.44
1:C:316:GLU:HG2	1:C:317:PRO:O	2.17	0.43
1:C:234:ARG:HD3	1:C:234:ARG:C	2.38	0.43
1:D:75:ARG:HB3	1:D:331:TRP:CZ2	2.53	0.43
1:A:20:VAL:HG13	1:A:214:LYS:O	2.19	0.43
1:A:183:VAL:O	1:A:229:CYS:HA	2.17	0.43
1:C:297:ILE:HA	5:C:3594:HOH:O	2.18	0.43
1:C:183:VAL:O	1:C:229:CYS:HA	2.19	0.43
1:C:312:LEU:HD23	1:C:318:LEU:HD21	2.01	0.43
1:A:274[A]:GLN:CD	5:A:5651:HOH:O	2.57	0.43
1:A:309:ASN:HB3	1:A:327:ALA:HA	2.01	0.42
1:A:332:GLU:HB2	5:A:5657:HOH:O	2.18	0.42
1:D:297:ILE:HA	5:D:4586:HOH:O	2.18	0.42
1:C:101:THR:HG22	5:C:3480:HOH:O	2.19	0.42
1:B:12[A]:GLU:HG2	1:B:13:ILE:N	2.34	0.42
1:C:210:LEU:HD21	1:D:119:ILE:HG21	2.01	0.42
1:C:297:ILE:HD12	1:C:298:GLY:N	2.34	0.42
1:A:138:LEU:HA	1:A:139:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:ASN:HB3	1:D:327:ALA:HA	2.01	0.42
1:D:186:LYS:HG2	1:D:232:ILE:HB	2.01	0.42
1:A:297:ILE:C	1:A:297:ILE:HD12	2.40	0.42
1:C:337:LEU:HD23	1:C:338:LEU:HD12	2.02	0.42
1:C:255:LYS:HD2	1:C:255:LYS:C	2.41	0.41
1:C:191:GLY:HA3	1:C:237:LYS:HZ3	1.83	0.41
1:B:302:GLU:HG3	5:B:2580:HOH:O	2.19	0.41
1:C:224:SER:CB	1:D:11:LYS:HE3	2.51	0.41
1:C:255:LYS:HD2	1:C:256:ALA:N	2.35	0.41
1:D:138:LEU:HA	1:D:139:PRO:HD3	1.89	0.41
1:C:309:ASN:O	1:C:322:LYS:HE2	2.20	0.41
1:C:159:TRP:CZ2	1:C:232:ILE:HD11	2.55	0.41
1:C:237:LYS:CE	1:C:237:LYS:H	2.31	0.41
1:C:309:ASN:HB3	1:C:327:ALA:HA	2.03	0.41
1:A:26:PHE:CE2	1:A:128:LYS:HD3	2.56	0.41
1:C:322:LYS:NZ	5:C:3615:HOH:O	2.53	0.41
1:A:186:LYS:HD3	4:A:1396:PEP:O3P	2.21	0.41
1:C:15:GLU:H	1:C:15:GLU:CD	2.17	0.41
1:A:244:LYS:N	1:A:244:LYS:HD3	2.35	0.41
1:C:263:MET:HA	1:C:298:GLY:O	2.21	0.41
1:A:244:LYS:N	1:A:244:LYS:CD	2.84	0.40
1:C:205:ALA:HB1	1:C:206:PRO:HD2	2.03	0.40
1:B:75:ARG:HB3	1:B:331:TRP:CZ2	2.57	0.40
1:C:84:LYS:HD3	1:C:85:ASP:N	2.37	0.40
1:C:141:ALA:HB1	1:C:159:TRP:HE3	1.86	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	344/350 (98%)	334 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	344/350 (98%)	336 (98%)	8 (2%)	0	100	100
1	C	341/350 (97%)	329 (96%)	12 (4%)	0	100	100
1	D	342/350 (98%)	335 (98%)	6 (2%)	1 (0%)	46	25
All	All	1371/1400 (98%)	1334 (97%)	36 (3%)	1 (0%)	56	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	313	GLU

5.3.2 Protein sidechains

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	279/283 (99%)	273 (98%)	6 (2%)	60	35
1	B	279/283 (99%)	277 (99%)	2 (1%)	88	79
1	C	276/283 (98%)	269 (98%)	7 (2%)	55	30
1	D	277/283 (98%)	275 (99%)	2 (1%)	88	79
All	All	1111/1132 (98%)	1094 (98%)	17 (2%)	72	55

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	77	LEU
1	A	187	ASN
1	A	234	ARG
1	A	244	LYS
1	A	316	GLU
1	B	187	ASN
1	B	234	ARG
1	C	84	LYS
1	C	130	LEU

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Mol	Chain	Res	Type
1	C	234	ARG
1	C	237	LYS
1	C	255	LYS
1	C	273	LYS
1	C	346	LYS
1	D	86	GLU
1	D	234	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	261	GLN
1	B	34	ASN
1	B	50	ASN
1	B	254	ASN
1	C	34	ASN
1	C	50	ASN
1	C	134	ASN
1	C	343	ASN
1	D	34	ASN
1	D	50	ASN
1	D	254	ASN
1	D	261	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 (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
4	PEP	A	1396	-	5,9,9	1.32	0	8,13,13	2.48	4 (50%)
3	SO4	A	5353	-	4,4,4	0.21	0	6,6,6	0.06	0
3	SO4	A	5356	-	4,4,4	0.29	0	6,6,6	0.15	0
4	PEP	B	1397	-	5,9,9	1.36	1 (20%)	8,13,13	2.34	4 (50%)
3	SO4	B	2353	-	4,4,4	0.21	0	6,6,6	0.06	0
3	SO4	B	2356	-	4,4,4	0.32	0	6,6,6	0.16	0
4	PEP	C	1398	-	5,9,9	1.37	0	8,13,13	2.39	4 (50%)
3	SO4	C	3353	-	4,4,4	0.20	0	6,6,6	0.07	0
3	SO4	C	3356	-	4,4,4	0.32	0	6,6,6	0.10	0
4	PEP	D	1399	-	5,9,9	1.47	1 (20%)	8,13,13	2.38	4 (50%)
3	SO4	D	4353	-	4,4,4	0.21	0	6,6,6	0.07	0
3	SO4	D	4356	-	4,4,4	0.31	0	6,6,6	0.10	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
4	PEP	A	1396	-	-	0/5/9/9	0/0/0/0
3	SO4	A	5353	-	-	0/0/0/0	0/0/0/0
3	SO4	A	5356	-	-	0/0/0/0	0/0/0/0
4	PEP	B	1397	-	-	0/5/9/9	0/0/0/0
3	SO4	B	2353	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2356	-	-	0/0/0/0	0/0/0/0
4	PEP	C	1398	-	-	0/5/9/9	0/0/0/0
3	SO4	C	3353	-	-	0/0/0/0	0/0/0/0
3	SO4	C	3356	-	-	0/0/0/0	0/0/0/0
4	PEP	D	1399	-	-	0/5/9/9	0/0/0/0
3	SO4	D	4353	-	-	0/0/0/0	0/0/0/0
3	SO4	D	4356	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1397	PEP	C3-C2	2.01	1.37	1.33
4	D	1399	PEP	C3-C2	2.13	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1398	PEP	O2-C2-C3	-3.22	118.21	124.73
4	D	1399	PEP	O2-C2-C3	-3.12	118.43	124.73
4	A	1396	PEP	O2-C2-C3	-3.04	118.59	124.73
4	B	1397	PEP	O2-C2-C3	-2.79	119.09	124.73
4	B	1397	PEP	O3P-P-O2P	2.12	115.45	107.38
4	A	1396	PEP	O3P-P-O2P	2.25	115.94	107.38
4	C	1398	PEP	O3P-P-O2P	2.27	116.03	107.38
4	D	1399	PEP	O3P-P-O2P	2.29	116.11	107.38
4	D	1399	PEP	P-O2-C2	2.64	128.84	122.96
4	C	1398	PEP	P-O2-C2	2.71	128.99	122.96
4	B	1397	PEP	P-O2-C2	3.22	130.12	122.96
4	A	1396	PEP	P-O2-C2	3.45	130.63	122.96
4	B	1397	PEP	C1-C2-C3	4.45	128.85	120.97
4	C	1398	PEP	C1-C2-C3	4.54	129.00	120.97
4	A	1396	PEP	C1-C2-C3	4.55	129.03	120.97
4	D	1399	PEP	C1-C2-C3	4.62	129.14	120.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1396	PEP	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	343/350 (98%)	0.36	17 (4%)	32	38	19, 30, 43, 67	0
1	B	343/350 (98%)	-0.05	5 (1%)	76	82	13, 20, 31, 47	0
1	C	343/350 (98%)	0.69	28 (8%)	14	18	23, 34, 49, 69	0
1	D	343/350 (98%)	0.45	29 (8%)	13	16	19, 29, 49, 64	0
All	All	1372/1400 (98%)	0.37	79 (5%)	26	31	13, 29, 46, 69	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	315	GLY	8.8
1	D	350	GLY	7.6
1	A	350	GLY	7.5
1	C	350	GLY	6.9
1	C	314	SER	6.7
1	A	316	GLU	6.4
1	A	315	GLY	6.4
1	A	313	GLU	6.3
1	C	316	GLU	5.9
1	D	315	GLY	5.4
1	B	8	LEU	5.4
1	A	314	SER	5.3
1	C	313	GLU	5.1
1	D	313	GLU	5.1
1	C	317	PRO	5.0
1	C	8	LEU	5.0
1	D	314	SER	4.8
1	B	350	GLY	4.7
1	D	8	LEU	4.5
1	C	273	LYS	4.3
1	A	30[A]	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	49	GLY	4.2
1	A	317	PRO	4.2
1	C	291	GLY	3.6
1	D	11	LYS	3.6
1	A	237	LYS	3.5
1	C	287	GLN	3.5
1	D	316	GLU	3.4
1	D	255	LYS	3.4
1	D	260	ALA	3.2
1	C	11	LYS	3.2
1	C	84	LYS	3.1
1	A	49	GLY	3.0
1	C	81	GLU	3.0
1	D	237	LYS	3.0
1	D	48	LYS	2.9
1	C	332	GLU	2.9
1	C	238	GLU	2.9
1	C	190	ASP	2.9
1	D	251	GLU	2.8
1	C	237	LYS	2.8
1	D	346	LYS	2.7
1	D	244	LYS	2.7
1	A	11	LYS	2.7
1	A	274[A]	GLN	2.7
1	A	50	ASN	2.6
1	C	292	GLY	2.6
1	D	294	LYS	2.6
1	C	290	ALA	2.5
1	D	190	ASP	2.5
1	B	313	GLU	2.5
1	D	41	LYS	2.5
1	A	8	LEU	2.5
1	C	50	ASN	2.4
1	B	12[A]	GLU	2.4
1	D	246	VAL	2.3
1	D	349	ARG	2.3
1	D	345	VAL	2.3
1	D	12	GLU	2.2
1	D	347	ALA	2.2
1	C	10	ILE	2.2
1	B	315	GLY	2.2
1	C	51	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	21	ALA	2.2
1	C	329	ILE	2.2
1	D	254	ASN	2.2
1	C	346	LYS	2.1
1	A	238	GLU	2.1
1	C	276	LYS	2.1
1	D	287	GLN	2.1
1	D	292	GLY	2.1
1	A	84	LYS	2.0
1	C	285	VAL	2.0
1	A	254	ASN	2.0
1	C	283	ALA	2.0
1	D	258	LEU	2.0
1	D	238	GLU	2.0
1	A	318	LEU	2.0
1	D	38	HIS	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	B	2353	5/5	0.96	0.12	3.03	28,30,35,38	0
3	SO4	A	5353	5/5	0.97	0.14	2.16	39,40,43,44	0
3	SO4	D	4353	5/5	0.97	0.11	1.31	38,39,41,42	0
3	SO4	C	3353	5/5	0.95	0.14	0.49	45,47,47,47	0
2	MN	B	351	1/1	0.99	0.09	0.20	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PEP	C	1398	10/10	0.94	0.10	-0.65	31,36,36,37	0
4	PEP	A	1396	10/10	0.98	0.08	-0.80	24,26,29,32	0
4	PEP	D	1399	10/10	0.97	0.07	-0.97	27,29,30,30	0
2	MN	D	351	1/1	0.99	0.06	-1.35	23,23,23,23	0
4	PEP	B	1397	10/10	0.99	0.06	-1.85	18,19,21,23	0
2	MN	C	351	1/1	0.97	0.05	-3.07	31,31,31,31	0
2	MN	A	351	1/1	0.99	0.04	-6.38	28,28,28,28	0
3	SO4	D	4356	5/5	0.95	0.31	-	49,49,51,53	0
3	SO4	A	5356	5/5	0.88	0.26	-	44,45,48,49	0
3	SO4	C	3356	5/5	0.89	0.29	-	47,48,50,51	0
3	SO4	B	2356	5/5	0.86	0.27	-	41,41,46,48	0

6.5 Other polymers

There are no such residues in this entry.