



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2017 – 11:08 PM EDT

PDB ID : 5FF9  
Title : Noroxomaritidine/Norcraftsodine Reductase in Complex with NADP<sup>+</sup> and tyramine  
Authors : Jez, J.M.; Holland, C.K.  
Deposited on : unknown  
Resolution : 1.81 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

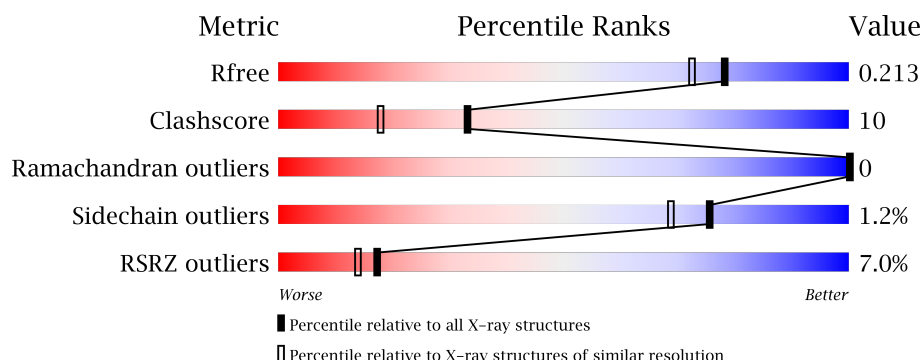
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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))
$R_{free}$	100719	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (1.84-1.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	257	<div> <div>9%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	B	257	<div> <div>4%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
1	C	257	<div> <div>11%</div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div>
1	D	257	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	302	-	-	-	X
3	SO4	B	303	-	-	-	X
3	SO4	B	304	-	-	-	X
3	SO4	B	305	-	-	X	-
3	SO4	D	302	-	-	X	-
3	SO4	D	303	-	-	-	X
4	AEF	B	302	-	-	-	X
4	AEF	D	301	-	-	-	X

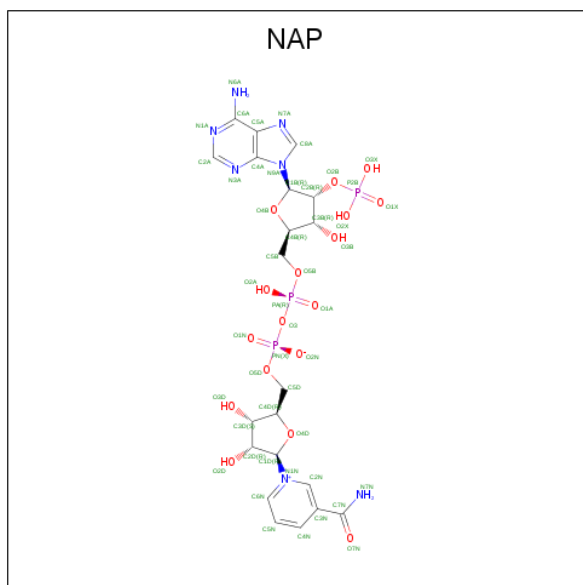


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Noroxomaritidine/Norcraugsodine Reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total 1857	C 1157	N 326	O 363	S 11	0	3	0
1	B	257	Total 1958	C 1221	N 341	O 385	S 11	0	6	0
1	C	245	Total 1853	C 1154	N 325	O 362	S 12	0	3	0
1	D	255	Total 1943	C 1218	N 336	O 377	S 12	0	7	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

*Continued on next page...*

Continued from previous page...

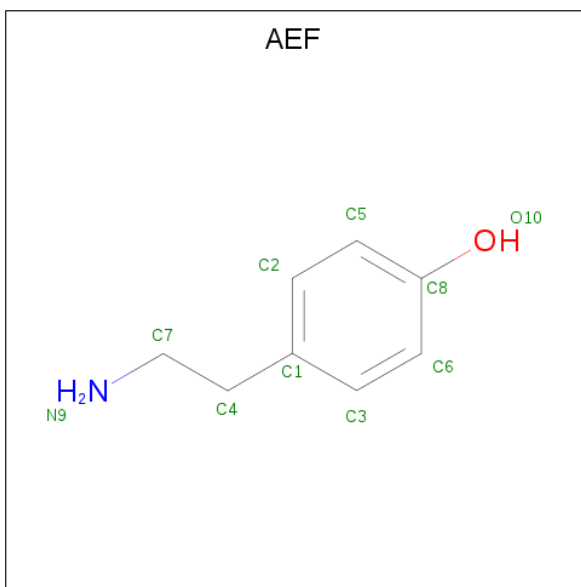
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is 4-(2-aminoethyl)phenol (three-letter code: AEF) (formula: C<sub>8</sub>H<sub>11</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			10	8	1	1		
4	D	1	Total	C	N	O	0	0
			10	8	1	1		

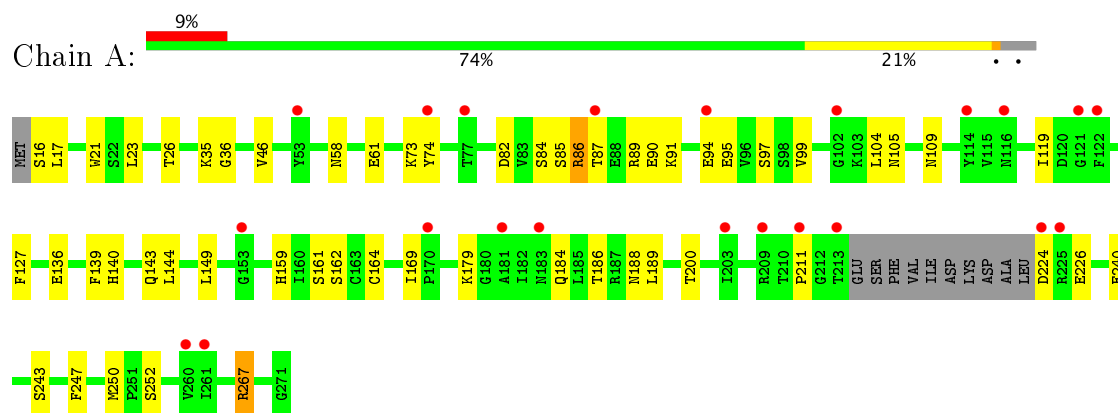
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	193	Total	O	0	0
			193	193		
5	C	54	Total	O	0	0
			54	54		
5	D	119	Total	O	0	0
			119	119		

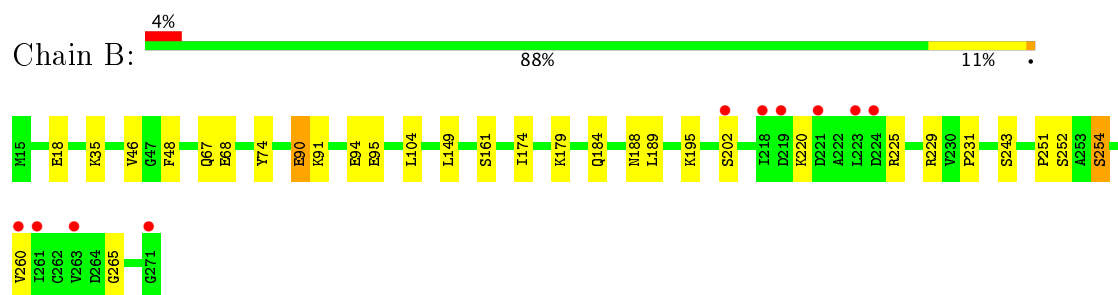
### 3 Residue-property plots [i](#)

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

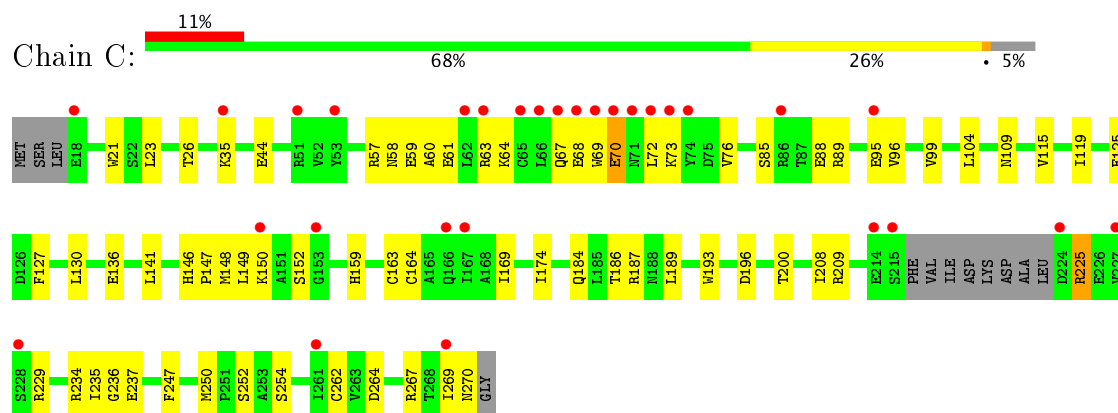
#### • Molecule 1: Noroxomaritidine/Norcraftsodine Reductase



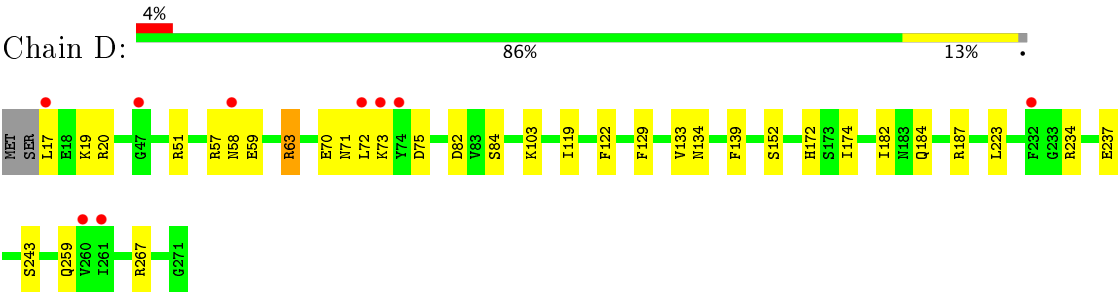
#### • Molecule 1: Noroxomaritidine/Norcraftsodine Reductase



#### • Molecule 1: Noroxomaritidine/Norcraftsodine Reductase



● Molecule 1: Noroxomaritidine/Norcraftsodine Reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.80 Å 86.96 Å 186.12 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.39 – 1.81 39.39 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.39-1.81) 95.9 (39.39-1.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 1.82 Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.184 , 0.214 0.181 , 0.213	Depositor DCC
$R_{free}$ test set	4391 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, SO4, AEF

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	0.35	0/1896	0.55	0/2565
1	B	0.46	1/2005 (0.0%)	0.56	0/2714
1	C	0.43	0/1892	0.62	1/2561 (0.0%)
1	D	0.48	0/1996	0.64	1/2702 (0.0%)
All	All	0.43	1/7789 (0.0%)	0.59	2/10542 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	GLU	C-N	-6.63	1.18	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	LEU	CA-CB-CG	10.37	139.15	115.30
1	C	225	ARG	NE-CZ-NH2	-6.00	117.30	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1857	0	1846	48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1958	0	1944	32	2
1	C	1853	0	1838	62	0
1	D	1943	0	1949	29	2
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	2	0
3	A	5	0	0	0	0
3	B	15	0	0	2	0
3	D	10	0	0	2	0
4	B	10	0	11	0	0
4	D	10	0	11	2	0
5	A	79	0	0	2	0
5	B	193	0	0	9	1
5	C	54	0	0	10	0
5	D	119	0	0	5	1
All	All	8250	0	7674	152	3

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 10.

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)
1:C:270:ASN:ND2	5:C:403:HOH:O	2.04	0.88
1:C:59:GLU:OE2	1:C:63:ARG:NH2	2.11	0.84
1:A:16:SER:N	5:A:401:HOH:O	2.12	0.82
1:D:70:GLU:O	1:D:73:LYS:N	2.13	0.82
1:C:234:ARG:NH1	5:C:401:HOH:O	1.96	0.79
1:C:95:GLU:O	1:C:99:VAL:HG23	1.82	0.79
1:C:35:LYS:NZ	1:C:61:GLU:OE1	2.14	0.79
1:C:254:SER:OG	5:C:402:HOH:O	1.98	0.79
1:A:119:ILE:HD13	1:C:189:LEU:HD23	1.66	0.76
1:D:84:SER:HB3	1:D:133[A]:VAL:HG12	1.68	0.76
1:B:95:GLU:OE2	5:B:401:HOH:O	2.05	0.74
3:B:305:SO4:S	5:B:402:HOH:O	2.46	0.74
1:C:68:GLU:O	1:C:72:LEU:HD23	1.89	0.72
1:C:235:ILE:O	5:C:401:HOH:O	2.07	0.71
1:C:149:LEU:O	1:C:152:SER:OG	2.08	0.71
1:C:270:ASN:O	5:C:404:HOH:O	2.07	0.71
1:B:251:PRO:O	1:B:254:SER:OG	2.08	0.71
1:C:150:LYS:NZ	5:C:405:HOH:O	2.25	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:305:SO4:O4	5:B:402:HOH:O	2.12	0.68
1:A:109:ASN:HD22	1:A:159:HIS:CD2	2.12	0.68
1:D:103:LYS:NZ	1:D:152:SER:HA	2.09	0.67
1:C:57:ARG:HD2	2:C:301:NAP:C6A	2.24	0.67
1:A:247:PHE:HA	1:A:250:MET:SD	2.35	0.67
1:A:58:ASN:OD1	1:A:61:GLU:HG3	1.95	0.67
1:C:209:ARG:NH2	1:C:237:GLU:OE2	2.28	0.66
1:A:140:HIS:CE1	1:A:144:LEU:HD11	2.30	0.66
1:D:172:HIS:NE2	4:D:301:AEF:H4	2.09	0.66
1:C:269:ILE:O	1:C:270:ASN:HB2	1.95	0.66
1:C:104:LEU:HB2	1:C:148:MET:HE2	1.77	0.65
1:A:23:LEU:O	1:A:26:THR:HG22	1.96	0.65
1:C:57:ARG:HD2	2:C:301:NAP:C5A	2.27	0.65
1:D:71:ASN:O	5:D:401:HOH:O	2.14	0.64
1:B:229:ARG:NH2	1:C:229:ARG:NH1	2.45	0.64
1:C:60:ALA:O	1:C:64:LYS:HG3	1.98	0.63
1:C:247:PHE:HA	1:C:250:MET:SD	2.39	0.63
1:D:103:LYS:HZ2	1:D:152:SER:HA	1.63	0.62
1:C:85:SER:OG	1:C:88:GLU:HG3	2.00	0.61
1:C:163[A]:CYS:SG	1:C:264:ASP:HB3	2.40	0.61
1:D:59:GLU:O	1:D:63:ARG:HG3	2.01	0.59
1:A:35:LYS:HD2	1:A:36:GLY:H	1.67	0.59
1:A:184:GLN:HE21	1:A:188:ASN:HD21	1.51	0.58
1:A:90:GLU:O	1:A:94:GLU:HG3	2.03	0.58
1:B:184:GLN:HE21	1:B:188:ASN:HD21	1.50	0.58
1:B:91:LYS:NZ	5:B:404:HOH:O	2.20	0.58
1:B:225:ARG:NH1	5:B:405:HOH:O	2.28	0.58
1:D:129:PHE:CE1	1:D:133[A]:VAL:HG11	2.39	0.58
1:A:26:THR:OG1	1:A:105:ASN:HB2	2.04	0.57
1:C:262:CYS:H	1:D:259:GLN:NE2	2.03	0.56
1:A:136:GLU:HB2	1:C:127:PHE:CZ	2.41	0.55
1:A:139:PHE:CE2	1:C:174:ILE:HD11	2.42	0.55
1:B:90:GLU:O	1:B:94:GLU:HG3	2.06	0.55
1:B:68:GLU:OE1	5:B:403:HOH:O	2.19	0.54
1:C:115:VAL:HB	1:C:130:LEU:HD11	1.89	0.54
1:D:103:LYS:HB3	1:D:103:LYS:NZ	2.22	0.53
1:B:229:ARG:NH2	1:C:229:ARG:HH12	2.06	0.53
1:A:224:ASP:N	5:A:405:HOH:O	2.40	0.53
1:A:82:ASP:OD1	1:A:84:SER:OG	2.22	0.53
1:D:184:GLN:HE21	1:D:187:ARG:HH21	1.55	0.53
1:C:109:ASN:HD22	1:C:159:HIS:CD2	2.27	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:GLN:NE2	1:C:187:ARG:HH11	2.08	0.52
1:C:67:GLN:O	1:C:70:GLU:HG3	2.10	0.52
1:A:184:GLN:HE21	1:A:188:ASN:ND2	2.08	0.52
1:C:252[A]:SER:HB2	1:D:243[A]:SER:HB3	1.92	0.52
1:C:23:LEU:O	1:C:26:THR:OG1	2.18	0.52
1:C:125:GLU:CD	1:C:125:GLU:H	2.13	0.51
1:A:35:LYS:HG3	1:A:211:PRO:HD2	1.93	0.51
1:B:91:LYS:NZ	5:B:401:HOH:O	2.39	0.51
1:A:127:PHE:CE2	1:C:136:GLU:HB2	2.45	0.51
1:A:35:LYS:CD	1:A:36:GLY:H	2.24	0.51
1:B:174:ILE:HD11	1:D:139:PHE:CE1	2.46	0.51
1:A:243:SER:HB2	1:B:252:SER:HB2	1.92	0.50
1:A:186:THR:HG23	1:A:200:THR:HG22	1.93	0.49
1:A:226:GLU:OE2	1:A:267:ARG:HD2	2.12	0.49
1:D:57:ARG:HG3	3:D:302:SO4:O3	2.12	0.49
1:B:195:LYS:NZ	5:B:407:HOH:O	2.34	0.49
1:A:136:GLU:HB2	1:C:127:PHE:CE1	2.48	0.49
1:C:164:CYS:HB3	1:C:169:ILE:HD12	1.94	0.49
1:C:58:ASN:ND2	1:C:61:GLU:OE2	2.45	0.49
1:D:237:GLU:OE2	5:D:403:HOH:O	2.20	0.49
1:A:35:LYS:HD2	1:A:36:GLY:N	2.28	0.48
1:B:46:VAL:HG11	1:B:74:TYR:CG	2.48	0.48
1:C:96:VAL:HG12	1:C:148:MET:HE1	1.95	0.48
3:D:302:SO4:O2	5:D:402:HOH:O	2.15	0.48
1:B:229:ARG:NH2	1:C:229:ARG:CZ	2.76	0.48
1:C:85:SER:CB	1:C:88:GLU:HG3	2.45	0.47
1:A:35:LYS:HG2	1:A:211:PRO:HG2	1.96	0.47
1:D:134:ASN:O	1:D:182[A]:ILE:HD11	2.14	0.47
1:A:87:THR:O	1:A:91:LYS:HG2	2.15	0.47
1:A:240:GLU:OE1	1:B:254:SER:HB2	2.15	0.47
1:C:69:TRP:CE3	1:C:76:VAL:HG11	2.50	0.46
4:D:301:AEF:H4A	5:D:508:HOH:O	2.15	0.46
1:B:225:ARG:HD2	5:B:405:HOH:O	2.14	0.46
1:C:72:LEU:O	1:C:73:LYS:HB2	2.15	0.46
1:B:161:SER:HA	1:B:179:LYS:HD2	1.97	0.46
1:B:229:ARG:NH2	5:C:403:HOH:O	2.48	0.45
1:C:236:GLY:HA2	5:C:401:HOH:O	2.16	0.45
1:C:186:THR:HG23	1:C:200:THR:HG22	1.99	0.45
1:A:252[A]:SER:HB2	1:B:243[A]:SER:HB3	1.98	0.45
1:B:189:LEU:HD23	1:D:119:ILE:HD13	1.99	0.45
1:B:35:LYS:HG2	2:B:301:NAP:H3B	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:PHE:CD1	1:D:174:ILE:HD12	2.52	0.45
1:D:103:LYS:HB3	1:D:103:LYS:HZ2	1.81	0.45
1:B:161:SER:O	2:B:301:NAP:H6N	2.17	0.44
1:A:140:HIS:HA	1:A:143:GLN:HE21	1.82	0.44
1:B:184:GLN:HE21	1:B:188:ASN:ND2	2.13	0.44
1:A:86:ARG:O	1:A:90:GLU:HG3	2.18	0.44
1:A:35:LYS:CG	1:A:211:PRO:HG2	2.47	0.44
1:D:51:ARG:HG2	1:D:75:ASP:OD2	2.18	0.44
1:B:18:GLU:H	1:B:18:GLU:CD	2.21	0.43
1:D:184:GLN:NE2	1:D:187:ARG:HE	2.16	0.43
1:B:202[A]:SER:HB3	1:B:260:VAL:HG22	2.01	0.43
1:A:127:PHE:CZ	1:C:136:GLU:HB2	2.53	0.43
1:C:146:HIS:HB3	1:C:147:PRO:HD3	1.99	0.43
1:B:104:LEU:O	1:B:149:LEU:HA	2.19	0.43
1:C:44:GLU:OE2	1:D:20:ARG:NH2	2.51	0.43
1:A:35:LYS:HA	1:A:35:LYS:HD2	1.37	0.43
1:D:57:ARG:HG2	1:D:82:ASP:HA	1.99	0.43
1:C:150:LYS:HD2	5:C:405:HOH:O	2.19	0.43
1:A:85:SER:O	1:A:89:ARG:HG3	2.19	0.42
1:A:189:LEU:HD23	1:C:119:ILE:HD13	2.00	0.42
1:A:252[B]:SER:HB3	1:B:243[B]:SER:HB2	2.02	0.42
1:D:71:ASN:OD1	1:D:71:ASN:N	2.51	0.42
1:A:95:GLU:O	1:A:99:VAL:HG23	2.19	0.42
1:C:89:ARG:HG2	1:C:141:LEU:HG	2.01	0.42
1:C:262:CYS:HB2	1:D:259:GLN:OE1	2.20	0.42
1:A:104:LEU:O	1:A:149:LEU:HD23	2.20	0.42
1:C:146:HIS:HB2	1:C:193:TRP:CH2	2.55	0.42
1:C:67:GLN:HA	1:C:70:GLU:CG	2.50	0.42
1:C:150:LYS:HD3	1:C:196:ASP:HB3	2.01	0.41
1:A:17:LEU:HD11	1:B:48:PHE:CZ	2.55	0.41
1:A:161:SER:OG	1:A:162:SER:N	2.52	0.41
1:A:23:LEU:HB3	1:A:26:THR:HG21	2.01	0.41
1:B:174:ILE:HD11	1:D:139:PHE:CZ	2.55	0.41
1:C:150:LYS:HD2	1:C:150:LYS:O	2.19	0.41
1:A:73:LYS:HB3	1:A:73:LYS:HE3	1.85	0.41
1:A:161:SER:HA	1:A:179:LYS:HD2	2.03	0.41
1:A:164:CYS:HB3	1:A:169:ILE:HD12	2.02	0.41
1:C:234:ARG:HD2	5:C:401:HOH:O	2.20	0.41
1:C:21:TRP:HA	1:C:250:MET:CE	2.50	0.41
1:D:223:LEU:HD12	1:D:223:LEU:HA	1.88	0.41
1:A:162:SER:HB2	2:A:301:NAP:H6N	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LEU:HA	1:D:17:LEU:HD12	1.88	0.41
1:A:46:VAL:HG11	1:A:74:TYR:CG	2.56	0.40
1:C:125:GLU:N	1:C:125:GLU:CD	2.74	0.40
1:C:104:LEU:O	1:C:149:LEU:HA	2.21	0.40
1:C:184:GLN:HE21	1:C:187:ARG:HH11	1.69	0.40
1:C:208:ILE:HD13	1:C:236:GLY:HA3	2.03	0.40
1:D:19:LYS:HD3	5:D:452:HOH:O	2.21	0.40
1:C:264:ASP:HB2	1:C:267:ARG:HB3	2.02	0.40
1:A:21:TRP:C	1:A:250:MET:HE3	2.42	0.40
1:B:231:PRO:HD2	1:B:265:GLY:O	2.21	0.40
1:A:252[A]:SER:HB2	1:B:243[A]:SER:CB	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLN:OE1	1:D:58:ASN:ND2[4_545]	1.64	0.56
1:B:67:GLN:NE2	1:D:58:ASN:ND2[4_545]	1.93	0.27
5:B:468:HOH:O	5:D:461:HOH:O[4_545]	2.16	0.04

## 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	245/257 (95%)	240 (98%)	5 (2%)	0	100	100
1	B	261/257 (102%)	257 (98%)	4 (2%)	0	100	100
1	C	244/257 (95%)	236 (97%)	8 (3%)	0	100	100
1	D	260/257 (101%)	254 (98%)	6 (2%)	0	100	100
All	All	1010/1028 (98%)	987 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	203/210 (97%)	200 (98%)	3 (2%)	70	60
1	B	215/210 (102%)	213 (99%)	2 (1%)	82	77
1	C	203/210 (97%)	201 (99%)	2 (1%)	80	74
1	D	214/210 (102%)	211 (99%)	3 (1%)	71	63
All	All	835/840 (99%)	825 (99%)	10 (1%)	75	69

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	97	SER
1	A	267	ARG
1	B	220	LYS
1	B	254	SER
1	C	70	GLU
1	C	225	ARG
1	D	63	ARG
1	D	234	ARG
1	D	267	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	143	GLN
1	A	159	HIS
1	A	188	ASN
1	A	270	ASN
1	B	39	HIS
1	B	109	ASN
1	B	159	HIS
1	B	188	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	101	ASN
1	C	143	GLN
1	C	159	HIS
1	C	166	GLN
1	C	184	GLN
1	D	184	GLN
1	D	197	ASN
1	D	259	GLN
1	D	270	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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	$\# Z  > 2$
2	NAP	A	301	-	44,52,52	1.12	2 (4%)	51,80,80	1.46	8 (15%)
3	SO4	A	302	-	4,4,4	0.19	0	6,6,6	0.11	0
2	NAP	B	301	-	44,52,52	1.60	10 (22%)	51,80,80	1.39	4 (7%)
4	AEF	B	302	-	10,10,10	2.25	6 (60%)	12,12,12	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	303	-	4,4,4	0.28	0	6,6,6	0.26	0
3	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.10	0
3	SO4	B	305	-	4,4,4	0.17	0	6,6,6	0.27	0
2	NAP	C	301	-	44,52,52	1.19	3 (6%)	51,80,80	1.50	7 (13%)
4	AEF	D	301	-	10,10,10	2.36	6 (60%)	12,12,12	0.68	0
3	SO4	D	302	-	4,4,4	0.17	0	6,6,6	0.06	0
3	SO4	D	303	-	4,4,4	0.13	0	6,6,6	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	NAP	A	301	-	-	0/27/67/67	0/5/5/5
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	NAP	B	301	-	-	0/27/67/67	0/5/5/5
4	AEF	B	302	-	-	0/3/3/3	0/1/1/1
3	SO4	B	303	-	-	0/0/0/0	0/0/0/0
3	SO4	B	304	-	-	0/0/0/0	0/0/0/0
3	SO4	B	305	-	-	0/0/0/0	0/0/0/0
2	NAP	C	301	-	-	0/27/67/67	0/5/5/5
4	AEF	D	301	-	-	0/3/3/3	0/1/1/1
3	SO4	D	302	-	-	0/0/0/0	0/0/0/0
3	SO4	D	303	-	-	0/0/0/0	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	P2B-O2X	-3.34	1.41	1.54
2	C	301	NAP	C2D-C1D	-3.11	1.48	1.53
2	B	301	NAP	O7N-C7N	-3.06	1.17	1.24
2	B	301	NAP	PN-O2N	-2.86	1.40	1.55
2	B	301	NAP	P2B-O1X	-2.71	1.41	1.50
2	B	301	NAP	P2B-O3X	-2.62	1.44	1.54
2	B	301	NAP	C5A-N7A	-2.61	1.30	1.39
2	B	301	NAP	PA-O1A	-2.59	1.41	1.50
2	B	301	NAP	PA-O2A	-2.26	1.43	1.55
2	C	301	NAP	C5A-N7A	-2.25	1.31	1.39
2	C	301	NAP	PA-O2A	-2.14	1.44	1.55
2	A	301	NAP	P2B-O3X	-2.10	1.46	1.54
2	A	301	NAP	O7N-C7N	-2.09	1.19	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C4A-N3A	-2.05	1.32	1.35
4	D	301	AEF	C6-C8	2.07	1.43	1.38
2	B	301	NAP	C5A-C4A	2.10	1.45	1.40
4	B	302	AEF	C6-C8	2.22	1.43	1.38
4	B	302	AEF	C3-C1	2.54	1.44	1.38
4	B	302	AEF	C2-C5	2.58	1.43	1.38
4	B	302	AEF	C2-C1	2.59	1.44	1.38
4	D	301	AEF	C2-C1	2.72	1.44	1.38
4	D	301	AEF	C3-C1	2.91	1.44	1.38
4	B	302	AEF	C3-C6	3.05	1.44	1.38
4	D	301	AEF	C2-C5	3.13	1.44	1.38
4	D	301	AEF	C3-C6	3.17	1.44	1.38
4	D	301	AEF	C5-C8	3.88	1.46	1.38
4	B	302	AEF	C5-C8	4.03	1.46	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAP	N3A-C2A-N1A	-5.71	123.89	128.86
2	C	301	NAP	N3A-C2A-N1A	-4.99	124.51	128.86
2	B	301	NAP	N3A-C2A-N1A	-4.95	124.55	128.86
2	C	301	NAP	O2X-P2B-O2B	-3.37	90.69	106.00
2	C	301	NAP	O4B-C1B-C2B	-2.87	101.57	106.59
2	A	301	NAP	O2X-P2B-O2B	-2.87	92.95	106.00
2	B	301	NAP	C4A-C5A-N7A	-2.77	106.74	109.41
2	A	301	NAP	C4A-C5A-N7A	-2.57	106.92	109.41
2	C	301	NAP	C4A-C5A-N7A	-2.30	107.19	109.41
2	A	301	NAP	C1B-N9A-C4A	-2.09	123.02	126.64
2	C	301	NAP	C3B-C2B-C1B	-2.09	98.67	102.75
2	A	301	NAP	C3B-C2B-C1B	-2.00	98.83	102.75
2	B	301	NAP	O5B-C5B-C4B	2.05	116.27	109.00
2	A	301	NAP	N6A-C6A-N1A	2.11	122.95	118.77
2	A	301	NAP	C2A-N1A-C6A	2.11	122.46	118.77
2	A	301	NAP	O3X-P2B-O2X	2.40	117.29	107.61
2	C	301	NAP	O2A-PA-O1A	2.81	126.84	112.28
2	C	301	NAP	O3X-P2B-O2X	3.11	120.18	107.61
2	B	301	NAP	N6A-C6A-N1A	3.34	125.38	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	1	0
2	B	301	NAP	2	0
3	B	305	SO4	2	0
2	C	301	NAP	2	0
4	D	301	AEF	2	0
3	D	302	SO4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	90:GLU	C	91:LYS	N	1.18

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	246/257 (95%)	0.58	22 (8%) 10 8	27, 47, 63, 71	1 (0%)
1	B	257/257 (100%)	0.02	10 (3%) 40 35	16, 25, 52, 75	0
1	C	245/257 (95%)	0.77	29 (11%) 5 4	35, 53, 74, 88	0
1	D	255/257 (99%)	0.12	9 (3%) 44 39	18, 36, 65, 78	0
All	All	1003/1028 (97%)	0.37	70 (6%) 17 14	16, 42, 66, 88	1 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72	LEU	6.4
1	C	224	ASP	6.1
1	B	218	ILE	5.9
1	D	72	LEU	5.0
1	C	74	TYR	5.0
1	A	260	VAL	4.0
1	D	58	ASN	3.8
1	B	224	ASP	3.8
1	C	73	LYS	3.8
1	C	63	ARG	3.7
1	D	73	LYS	3.5
1	A	213	THR	3.5
1	B	221	ASP	3.4
1	A	224	ASP	3.4
1	B	261	ILE	3.4
1	D	74	TYR	3.4
1	C	53	TYR	3.3
1	C	65	CYS	3.3
1	C	67	GLN	3.3
1	C	71	ASN	3.3
1	D	260	VAL	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	214	GLU	3.3
1	D	17	LEU	3.1
1	C	18	GLU	3.1
1	C	66	LEU	3.0
1	C	69	TRP	3.0
1	C	153	GLY	3.0
1	A	114	TYR	2.9
1	A	121	GLY	2.8
1	C	51	ARG	2.7
1	A	170	PRO	2.7
1	C	70	GLU	2.7
1	B	260	VAL	2.7
1	D	47	GLY	2.6
1	D	232	PHE	2.6
1	C	95	GLU	2.6
1	C	150	LYS	2.5
1	A	122	PHE	2.5
1	C	215	SER	2.5
1	A	102	GLY	2.5
1	A	181	ALA	2.5
1	A	153	GLY	2.5
1	C	269	ILE	2.5
1	B	223	LEU	2.5
1	B	219	ASP	2.4
1	B	271	GLY	2.4
1	A	183	ASN	2.4
1	A	225	ARG	2.4
1	A	74	TYR	2.4
1	B	202[A]	SER	2.4
1	A	261	ILE	2.4
1	C	86	ARG	2.3
1	A	203	ILE	2.3
1	A	87	THR	2.3
1	C	68	GLU	2.3
1	C	261	ILE	2.3
1	C	62	LEU	2.3
1	A	209	ARG	2.3
1	A	77	THR	2.3
1	C	166	GLN	2.2
1	C	167	ILE	2.2
1	A	94	GLU	2.2
1	A	53	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	227	VAL	2.2
1	C	228	SER	2.1
1	A	116	ASN	2.1
1	D	261	ILE	2.1
1	C	35	LYS	2.1
1	B	263	VAL	2.1
1	A	211	PRO	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	B	304	5/5	0.98	0.40	7.29	31,34,43,46	5
3	SO4	D	303	5/5	0.86	0.44	7.19	40,50,55,57	5
3	SO4	A	302	5/5	0.91	0.50	5.80	35,49,54,54	5
4	AEF	B	302	10/10	0.79	0.18	3.08	50,54,65,72	0
3	SO4	B	303	5/5	0.87	0.12	2.72	23,37,42,45	5
4	AEF	D	301	10/10	0.89	0.15	2.07	26,32,39,63	0
3	SO4	D	302	5/5	0.93	0.17	0.52	44,47,55,56	5
2	NAP	A	301	48/48	0.91	0.12	-0.14	23,35,40,49	48
2	NAP	C	301	48/48	0.90	0.13	-0.22	24,32,43,51	48
2	NAP	B	301	48/48	0.98	0.07	-0.63	14,18,20,27	0
3	SO4	B	305	5/5	0.93	0.16	-	36,40,45,51	5

## 6.5 Other polymers

There are no such residues in this entry.