



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 07:36 pm GMT

PDB ID : 5F1W  
Title : Crystal structure of the enantiomer of a macrocyclic peptide containing fragments from alpha synuclein 36-55  
Authors : Salveson, P.J.; Spencer, R.K.; Nowick, J.S.  
Deposited on : 2015-11-30  
Resolution : 2.16 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.

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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	:	trunk28620
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)	:	recalc28949

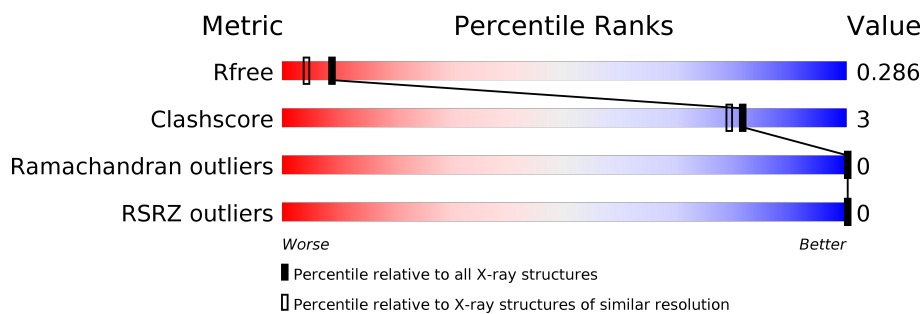
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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	16	
1	B	16	
1	C	16	
1	D	16	
1	E	16	
1	F	16	

## 2 Entry composition [i](#)

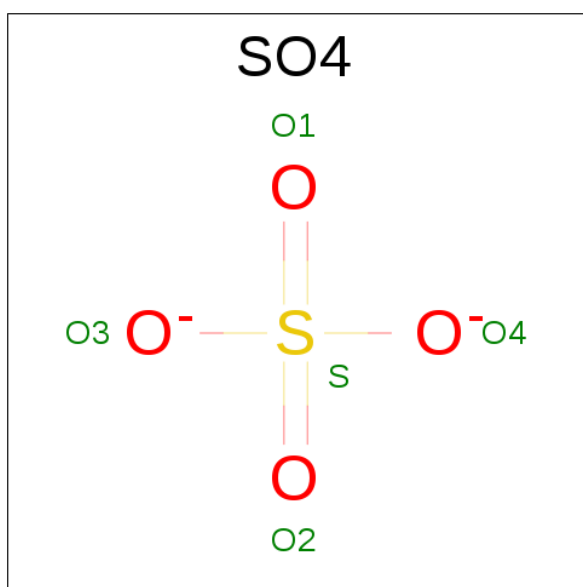
There are 4 unique types of molecules in this entry. The entry contains 1518 atoms, of which 764 are hydrogens and 0 are deuteriums.

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 (with D amino acids) called Macrocytic peptide.

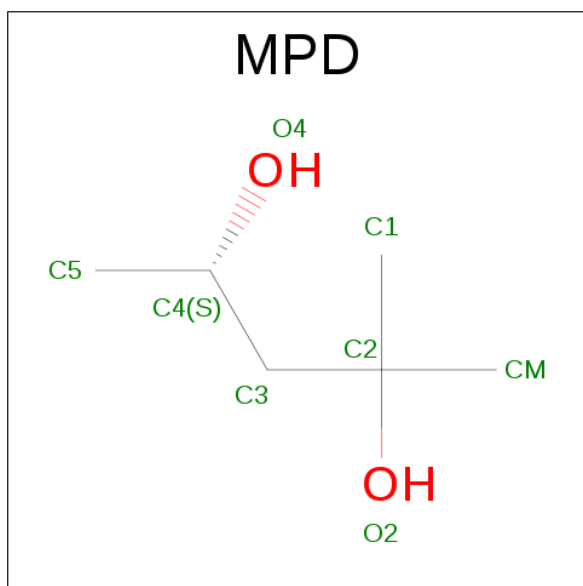
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	16	Total	C	H	I	N	O	0	0	0
			236	74	123	1	20	18			
1	B	16	Total	C	H	I	N	O	0	0	0
			235	74	122	1	20	18			
1	C	16	Total	C	H	I	N	O	0	0	0
			235	74	122	1	20	18			
1	D	16	Total	C	H	I	N	O	0	0	0
			236	74	123	1	20	18			
1	E	16	Total	C	H	I	N	O	0	0	0
			236	74	123	1	20	18			
1	F	16	Total	C	H	I	N	O	0	0	0
			236	74	123	1	20	18			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			22	6	14	2		
3	C	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	8	Total	O	0	0
			8	8		
4	C	7	Total	O	0	0
			7	7		
4	D	13	Total	O	0	0
			13	13		
4	E	6	Total	O	0	0
			6	6		
4	F	11	Total	O	0	0
			11	11		

### 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: Macrocyclic peptide

Chain A: 



- Molecule 1: Macrocyclic peptide

Chain B: 



- Molecule 1: Macrocyclic peptide

Chain C: 



- Molecule 1: Macrocyclic peptide

Chain D: 

There are no outlier residues recorded for this chain.

- Molecule 1: Macrocyclic peptide

Chain E: 



- Molecule 1: Macrocyclic peptide

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.91Å 77.91Å 77.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.84 – 2.16 34.84 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.84-2.16) 96.7 (34.84-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.223 , 0.283 0.234 , 0.286	Depositor DCC
$R_{free}$ test set	856 reflections (11.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.076 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	1518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: MPD, DTH, IOY, DLE, DAL, MV9, DVA, DSN, SO4, DHI, ORD

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	0.23	0/6	0.71	0/4
1	B	0.21	0/6	0.40	0/4
1	C	0.26	0/6	0.34	0/4
1	D	0.23	0/6	0.81	0/4
1	E	0.25	0/6	0.51	0/4
1	F	0.27	0/6	0.48	0/4
All	All	0.24	0/36	0.57	0/24

There are no bond length outliers.

There are no bond angle outliers.

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	113	123	99	1	0
1	B	113	122	100	1	0
1	C	113	122	100	1	0
1	D	113	123	100	0	0
1	E	113	123	102	1	0
1	F	113	123	99	1	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	14	14	0	0
3	C	8	14	14	0	0
4	A	10	0	0	0	0
4	B	8	0	0	0	0
4	C	7	0	0	1	0
4	D	13	0	0	0	0
4	E	6	0	0	0	0
4	F	11	0	0	0	0
All	All	754	764	628	4	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 3.

All (4) 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:8:DSN:OG	4:C:201:HOH:O	2.18	0.50
1:A:16:DVA:HG12	1:A:16:DVA:O	2.14	0.48
1:B:12:GLY:HA3	1:E:5:IOY:HD1	1.99	0.44
1:F:5:IOY:CD2	1:F:5:IOY:N	2.84	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

84 non-standard protein/DNA/RNA residues 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$
1	ORD	A	1	1	7,7,8	1.69	1 (14%)	4,7,9	0.74	0
1	DVA	A	10	1	6,6,7	0.76	0	6,7,9	0.90	0
1	DHI	A	11	1	7,10,11	0.97	0	3,12,14	0.92	0
1	MV9	A	13	1	7,7,8	0.61	0	7,8,10	1.21	1 (14%)
1	DAL	A	14	1	4,4,5	1.14	1 (25%)	1,4,6	0.10	0
1	DTH	A	15	1	6,6,7	1.66	1 (16%)	6,7,9	1.20	1 (16%)
1	DVA	A	16	1	6,6,7	1.21	1 (16%)	6,7,9	1.03	1 (16%)
1	DAL	A	2	1	4,4,5	1.19	1 (25%)	1,4,6	0.22	0
1	DVA	A	3	1	6,6,7	1.02	1 (16%)	6,7,9	0.88	0
1	DLE	A	4	1	7,7,8	0.80	0	6,8,10	0.64	0
1	IOY	A	5	1	12,12,13	1.69	3 (25%)	14,15,17	0.92	0
1	DVA	A	6	1	6,6,7	0.91	0	6,7,9	0.88	0
1	DSN	A	8	1	5,5,6	5.84	2 (40%)	1,5,7	1.36	0
1	ORD	A	9	1	7,7,8	1.43	1 (14%)	4,7,9	0.94	0
1	ORD	B	1	1	7,7,8	1.71	1 (14%)	4,7,9	0.69	0
1	DVA	B	10	1	6,6,7	0.82	0	6,7,9	0.95	0
1	DHI	B	11	1	7,10,11	0.88	0	3,12,14	1.10	0
1	MV9	B	13	1	7,7,8	0.62	0	7,8,10	1.22	1 (14%)
1	DAL	B	14	1	4,4,5	1.03	0	1,4,6	0.28	0
1	DTH	B	15	1	6,6,7	1.53	1 (16%)	6,7,9	1.33	1 (16%)
1	DVA	B	16	1	6,6,7	0.79	0	6,7,9	0.96	0
1	DAL	B	2	1	4,4,5	0.90	0	1,4,6	0.18	0
1	DVA	B	3	1	6,6,7	0.93	0	6,7,9	1.06	1 (16%)
1	DLE	B	4	1	7,7,8	0.75	0	6,8,10	0.58	0
1	IOY	B	5	1	12,12,13	1.65	3 (25%)	14,15,17	0.95	0
1	DVA	B	6	1	6,6,7	0.84	0	6,7,9	1.06	0
1	DSN	B	8	1	5,5,6	5.64	2 (40%)	1,5,7	1.29	0
1	ORD	B	9	1	7,7,8	1.60	1 (14%)	4,7,9	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	ORD	C	1	1	7,7,8	1.56	1 (14%)	4,7,9	0.70	0
1	DVA	C	10	1	6,6,7	0.85	0	6,7,9	0.92	0
1	DHI	C	11	1	6,10,11	1.00	0	5,12,14	1.29	1 (20%)
1	MV9	C	13	1	7,7,8	0.61	0	7,8,10	1.43	1 (14%)
1	DAL	C	14	1	4,4,5	1.02	0	1,4,6	0.17	0
1	DTH	C	15	1	6,6,7	1.54	1 (16%)	6,7,9	1.36	1 (16%)
1	DVA	C	16	1	6,6,7	0.80	0	6,7,9	0.90	0
1	DAL	C	2	1	4,4,5	1.02	0	1,4,6	0.19	0
1	DVA	C	3	1	6,6,7	0.90	0	6,7,9	1.04	1 (16%)
1	DLE	C	4	1	7,7,8	0.81	0	6,8,10	0.56	0
1	IOY	C	5	1	12,12,13	1.66	3 (25%)	14,15,17	0.92	0
1	DVA	C	6	1	6,6,7	0.88	0	6,7,9	1.04	0
1	DSN	C	8	1	5,5,6	5.74	2 (40%)	1,5,7	1.38	0
1	ORD	C	9	1	7,7,8	1.62	1 (14%)	4,7,9	0.47	0
1	ORD	D	1	1	7,7,8	1.69	1 (14%)	4,7,9	0.85	0
1	DVA	D	10	1	6,6,7	0.89	0	6,7,9	0.95	0
1	DHI	D	11	1	6,10,11	0.99	0	5,12,14	1.34	1 (20%)
1	MV9	D	13	1	7,7,8	0.60	0	7,8,10	1.34	1 (14%)
1	DAL	D	14	1	4,4,5	1.27	1 (25%)	1,4,6	0.13	0
1	DTH	D	15	1	6,6,7	1.74	1 (16%)	6,7,9	1.31	1 (16%)
1	DVA	D	16	1	6,6,7	0.95	0	6,7,9	1.08	1 (16%)
1	DAL	D	2	1	4,4,5	1.14	1 (25%)	1,4,6	0.20	0
1	DVA	D	3	1	6,6,7	0.96	1 (16%)	6,7,9	0.91	0
1	DLE	D	4	1	7,7,8	0.89	1 (14%)	6,8,10	0.62	0
1	IOY	D	5	1	12,12,13	1.69	3 (25%)	14,15,17	0.91	0
1	DVA	D	6	1	6,6,7	0.93	0	6,7,9	0.98	0
1	DSN	D	8	1	5,5,6	5.78	2 (40%)	1,5,7	1.33	0
1	ORD	D	9	1	7,7,8	1.46	1 (14%)	4,7,9	0.96	0
1	ORD	E	1	1	7,7,8	1.62	1 (14%)	4,7,9	0.86	0
1	DVA	E	10	1	6,6,7	0.94	0	6,7,9	1.09	0
1	DHI	E	11	1	6,10,11	1.12	1 (16%)	5,12,14	1.33	1 (20%)
1	MV9	E	13	1	7,7,8	0.56	0	7,8,10	1.42	1 (14%)
1	DAL	E	14	1	4,4,5	1.15	1 (25%)	1,4,6	0.18	0
1	DTH	E	15	1	6,6,7	1.60	1 (16%)	6,7,9	1.29	1 (16%)
1	DVA	E	16	1	6,6,7	0.93	0	6,7,9	1.09	0
1	DAL	E	2	1	4,4,5	1.15	1 (25%)	1,4,6	0.28	0
1	DVA	E	3	1	6,6,7	0.86	0	6,7,9	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DLE	E	4	1	7,7,8	0.83	0	6,8,10	0.58	0
1	IOY	E	5	1	12,12,13	1.73	4 (33%)	14,15,17	0.91	1 (7%)
1	DVA	E	6	1	6,6,7	0.98	1 (16%)	6,7,9	0.89	0
1	DSN	E	8	1	5,5,6	5.77	2 (40%)	1,5,7	1.41	0
1	ORD	E	9	1	7,7,8	1.59	1 (14%)	4,7,9	0.96	0
1	ORD	F	1	1	7,7,8	1.56	1 (14%)	4,7,9	0.74	0
1	DVA	F	10	1	6,6,7	0.93	0	6,7,9	0.99	0
1	DHI	F	11	1	6,10,11	1.07	0	5,12,14	1.29	1 (20%)
1	MV9	F	13	1	7,7,8	0.57	0	7,8,10	1.52	1 (14%)
1	DAL	F	14	1	4,4,5	1.01	0	1,4,6	0.28	0
1	DTH	F	15	1	6,6,7	1.53	1 (16%)	6,7,9	1.71	2 (33%)
1	DVA	F	16	1	6,6,7	0.83	0	6,7,9	0.88	0
1	DAL	F	2	1	4,4,5	1.06	0	1,4,6	0.20	0
1	DVA	F	3	1	6,6,7	0.89	0	6,7,9	0.97	0
1	DLE	F	4	1	7,7,8	0.71	0	6,8,10	0.54	0
1	IOY	F	5	1	12,12,13	1.74	4 (33%)	14,15,17	0.92	0
1	DVA	F	6	1	6,6,7	0.89	0	6,7,9	0.98	0
1	DSN	F	8	1	5,5,6	5.79	2 (40%)	1,5,7	1.47	0
1	ORD	F	9	1	7,7,8	1.56	1 (14%)	4,7,9	0.81	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
1	ORD	A	1	1	-	0/4/6/8	0/0/0/0
1	DVA	A	10	1	-	0/5/6/8	0/0/0/0
1	DHI	A	11	1	-	0/4/6/8	0/1/1/1
1	MV9	A	13	1	-	0/5/8/10	0/0/0/0
1	DAL	A	14	1	-	0/0/2/4	0/0/0/0
1	DTH	A	15	1	-	0/4/6/8	0/0/0/0
1	DVA	A	16	1	-	0/5/6/8	0/0/0/0
1	DAL	A	2	1	-	0/0/2/4	0/0/0/0
1	DVA	A	3	1	-	0/5/6/8	0/0/0/0
1	DLE	A	4	1	-	0/4/6/8	0/0/0/0
1	IOY	A	5	1	-	0/4/6/8	0/1/1/1
1	DVA	A	6	1	-	0/5/6/8	0/0/0/0
1	DSN	A	8	1	-	0/2/4/6	0/0/0/0
1	ORD	A	9	1	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ORD	B	1	1	-	0/4/6/8	0/0/0/0
1	DVA	B	10	1	-	0/5/6/8	0/0/0/0
1	DHI	B	11	1	-	0/4/6/8	0/1/1/1
1	MV9	B	13	1	-	0/5/8/10	0/0/0/0
1	DAL	B	14	1	-	0/0/2/4	0/0/0/0
1	DTH	B	15	1	-	0/4/6/8	0/0/0/0
1	DVA	B	16	1	-	0/5/6/8	0/0/0/0
1	DAL	B	2	1	-	0/0/2/4	0/0/0/0
1	DVA	B	3	1	-	0/5/6/8	0/0/0/0
1	DLE	B	4	1	-	0/4/6/8	0/0/0/0
1	IOY	B	5	1	-	0/4/6/8	0/1/1/1
1	DVA	B	6	1	-	0/5/6/8	0/0/0/0
1	DSN	B	8	1	-	0/2/4/6	0/0/0/0
1	ORD	B	9	1	-	0/4/6/8	0/0/0/0
1	ORD	C	1	1	-	0/4/6/8	0/0/0/0
1	DVA	C	10	1	-	0/5/6/8	0/0/0/0
1	DHI	C	11	1	-	0/3/6/8	0/1/1/1
1	MV9	C	13	1	-	0/5/8/10	0/0/0/0
1	DAL	C	14	1	-	0/0/2/4	0/0/0/0
1	DTH	C	15	1	-	0/4/6/8	0/0/0/0
1	DVA	C	16	1	-	0/5/6/8	0/0/0/0
1	DAL	C	2	1	-	0/0/2/4	0/0/0/0
1	DVA	C	3	1	-	0/5/6/8	0/0/0/0
1	DLE	C	4	1	-	0/4/6/8	0/0/0/0
1	IOY	C	5	1	-	0/4/6/8	0/1/1/1
1	DVA	C	6	1	-	0/5/6/8	0/0/0/0
1	DSN	C	8	1	-	0/2/4/6	0/0/0/0
1	ORD	C	9	1	-	0/4/6/8	0/0/0/0
1	ORD	D	1	1	-	0/4/6/8	0/0/0/0
1	DVA	D	10	1	-	0/5/6/8	0/0/0/0
1	DHI	D	11	1	-	0/3/6/8	0/1/1/1
1	MV9	D	13	1	-	0/5/8/10	0/0/0/0
1	DAL	D	14	1	-	0/0/2/4	0/0/0/0
1	DTH	D	15	1	-	0/4/6/8	0/0/0/0
1	DVA	D	16	1	-	0/5/6/8	0/0/0/0
1	DAL	D	2	1	-	0/0/2/4	0/0/0/0
1	DVA	D	3	1	-	0/5/6/8	0/0/0/0
1	DLE	D	4	1	-	0/4/6/8	0/0/0/0
1	IOY	D	5	1	-	0/4/6/8	0/1/1/1
1	DVA	D	6	1	-	0/5/6/8	0/0/0/0
1	DSN	D	8	1	-	0/2/4/6	0/0/0/0
1	ORD	D	9	1	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ORD	E	1	1	-	0/4/6/8	0/0/0/0
1	DVA	E	10	1	-	0/5/6/8	0/0/0/0
1	DHI	E	11	1	-	0/3/6/8	0/1/1/1
1	MV9	E	13	1	-	0/5/8/10	0/0/0/0
1	DAL	E	14	1	-	0/0/2/4	0/0/0/0
1	DTH	E	15	1	-	0/4/6/8	0/0/0/0
1	DVA	E	16	1	-	0/5/6/8	0/0/0/0
1	DAL	E	2	1	-	0/0/2/4	0/0/0/0
1	DVA	E	3	1	-	0/5/6/8	0/0/0/0
1	DLE	E	4	1	-	0/4/6/8	0/0/0/0
1	IOY	E	5	1	-	0/4/6/8	0/1/1/1
1	DVA	E	6	1	-	0/5/6/8	0/0/0/0
1	DSN	E	8	1	-	0/2/4/6	0/0/0/0
1	ORD	E	9	1	-	0/4/6/8	0/0/0/0
1	ORD	F	1	1	-	0/4/6/8	0/0/0/0
1	DVA	F	10	1	-	0/5/6/8	0/0/0/0
1	DHI	F	11	1	-	0/3/6/8	0/1/1/1
1	MV9	F	13	1	-	0/5/8/10	0/0/0/0
1	DAL	F	14	1	-	0/0/2/4	0/0/0/0
1	DTH	F	15	1	-	0/4/6/8	0/0/0/0
1	DVA	F	16	1	-	0/5/6/8	0/0/0/0
1	DAL	F	2	1	-	0/0/2/4	0/0/0/0
1	DVA	F	3	1	-	0/5/6/8	0/0/0/0
1	DLE	F	4	1	-	0/4/6/8	0/0/0/0
1	IOY	F	5	1	-	0/4/6/8	0/1/1/1
1	DVA	F	6	1	-	0/5/6/8	0/0/0/0
1	DSN	F	8	1	-	0/2/4/6	0/0/0/0
1	ORD	F	9	1	-	0/4/6/8	0/0/0/0

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	DSN	CA-C	-12.37	1.34	1.50
1	F	8	DSN	CA-C	-12.26	1.34	1.50
1	D	8	DSN	CA-C	-12.26	1.34	1.50
1	E	8	DSN	CA-C	-12.19	1.34	1.50
1	C	8	DSN	CA-C	-12.14	1.34	1.50
1	B	8	DSN	CA-C	-11.92	1.34	1.50
1	E	8	DSN	CA-N	-4.12	1.34	1.47
1	F	8	DSN	CA-N	-4.11	1.34	1.47
1	A	8	DSN	CA-N	-4.08	1.34	1.47
1	C	8	DSN	CA-N	-4.08	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	DSN	CA-N	-4.04	1.34	1.47
1	B	8	DSN	CA-N	-4.01	1.34	1.47
1	A	14	DAL	CA-C	2.01	1.52	1.50
1	E	5	IOY	CB-CG	2.05	1.56	1.51
1	D	2	DAL	CA-C	2.05	1.52	1.50
1	D	3	DVA	CA-C	2.06	1.53	1.50
1	E	11	DHI	CA-C	2.09	1.53	1.50
1	E	2	DAL	CA-C	2.09	1.53	1.50
1	E	14	DAL	CA-C	2.09	1.53	1.50
1	D	4	DLE	CA-C	2.13	1.53	1.50
1	B	5	IOY	O-C	2.16	1.29	1.19
1	C	5	IOY	O-C	2.18	1.29	1.19
1	A	2	DAL	CA-C	2.19	1.53	1.50
1	E	6	DVA	CA-C	2.19	1.53	1.50
1	F	5	IOY	O-C	2.21	1.29	1.19
1	E	5	IOY	O-C	2.21	1.29	1.19
1	D	5	IOY	O-C	2.22	1.29	1.19
1	F	5	IOY	CB-CG	2.23	1.56	1.51
1	A	5	IOY	O-C	2.23	1.29	1.19
1	A	3	DVA	CA-C	2.25	1.53	1.50
1	D	14	DAL	CA-C	2.33	1.53	1.50
1	A	16	DVA	CA-C	2.73	1.53	1.50
1	F	5	IOY	CE2-CZ	2.85	1.45	1.38
1	C	5	IOY	CE2-CZ	2.97	1.45	1.38
1	A	5	IOY	CE2-CZ	2.98	1.45	1.38
1	B	5	IOY	CE2-CZ	3.00	1.45	1.38
1	E	5	IOY	CE2-CZ	3.03	1.45	1.38
1	D	5	IOY	CE2-CZ	3.03	1.45	1.38
1	B	15	DTH	CA-C	3.41	1.54	1.50
1	C	15	DTH	CA-C	3.45	1.54	1.50
1	F	15	DTH	CA-C	3.47	1.54	1.50
1	B	5	IOY	CD1-CG	3.51	1.46	1.38
1	A	9	ORD	CA-C	3.55	1.54	1.50
1	C	5	IOY	CD1-CG	3.55	1.46	1.38
1	E	5	IOY	CD1-CG	3.61	1.46	1.38
1	A	5	IOY	CD1-CG	3.61	1.46	1.38
1	D	5	IOY	CD1-CG	3.62	1.46	1.38
1	D	9	ORD	CA-C	3.62	1.55	1.50
1	E	15	DTH	CA-C	3.63	1.55	1.50
1	F	5	IOY	CD1-CG	3.72	1.46	1.38
1	A	15	DTH	CA-C	3.78	1.55	1.50
1	F	9	ORD	CA-C	3.82	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1	ORD	CA-C	3.90	1.55	1.50
1	C	1	ORD	CA-C	3.94	1.55	1.50
1	E	1	ORD	CA-C	3.95	1.55	1.50
1	E	9	ORD	CA-C	3.98	1.55	1.50
1	D	15	DTH	CA-C	4.01	1.55	1.50
1	B	9	ORD	CA-C	4.02	1.55	1.50
1	A	1	ORD	CA-C	4.09	1.55	1.50
1	C	9	ORD	CA-C	4.10	1.55	1.50
1	D	1	ORD	CA-C	4.22	1.55	1.50
1	B	1	ORD	CA-C	4.22	1.55	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	15	DTH	O-C-CA	-2.95	118.28	125.15
1	F	13	MV9	CB-CA-C	-2.83	109.47	113.07
1	D	13	MV9	CB-CA-C	-2.81	109.50	113.07
1	E	13	MV9	CB-CA-C	-2.71	109.62	113.07
1	C	13	MV9	CB-CA-C	-2.50	109.88	113.07
1	D	15	DTH	O-C-CA	-2.49	119.33	125.15
1	F	15	DTH	C-CA-N	-2.48	104.85	109.86
1	E	5	IOY	CG-CB-CA	-2.41	109.43	114.29
1	A	13	MV9	CB-CA-C	-2.33	110.11	113.07
1	B	15	DTH	O-C-CA	-2.23	119.94	125.15
1	E	15	DTH	O-C-CA	-2.16	120.12	125.15
1	C	15	DTH	O-C-CA	-2.07	120.33	125.15
1	B	13	MV9	CB-CA-C	-2.04	110.47	113.07
1	C	3	DVA	O-C-CA	-2.04	120.40	125.15
1	D	16	DVA	O-C-CA	-2.01	120.45	125.15
1	A	15	DTH	O-C-CA	-2.01	120.45	125.15
1	B	3	DVA	O-C-CA	-2.00	120.48	125.15
1	A	16	DVA	O-C-CA	-2.00	120.48	125.15
1	C	11	DHI	CD2-NE2-CE1	2.02	108.87	105.75
1	F	11	DHI	CD2-NE2-CE1	2.04	108.91	105.75
1	E	11	DHI	CD2-NE2-CE1	2.06	108.94	105.75
1	D	11	DHI	CD2-NE2-CE1	2.10	109.00	105.75

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
1	A	16	DVA	1	0
1	C	8	DSN	1	0
1	E	5	IOY	1	0
1	F	5	IOY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	SO4	B	101	-	4,4,4	0.14	0	6,6,6	0.05	0
3	MPD	B	102	-	7,7,7	0.29	0	9,10,10	0.39	0
3	MPD	C	101	-	7,7,7	0.28	0	9,10,10	0.37	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	SO4	B	101	-	-	0/0/0/0	0/0/0/0
3	MPD	B	102	-	-	0/5/5/5	0/0/0/0
3	MPD	C	101	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

## 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	D	1
1	E	1
1	B	1
1	C	1
1	A	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	8:DSN	C	9:ORD	N	5.56
1	B	8:DSN	C	9:ORD	N	5.46
1	D	8:DSN	C	9:ORD	N	5.41
1	A	8:DSN	C	9:ORD	N	5.37
1	E	8:DSN	C	9:ORD	N	5.37
1	F	8:DSN	C	9:ORD	N	5.36

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	2/16 (12%)	0.05	0 100 100	30, 30, 30, 37	0
1	B	2/16 (12%)	-0.22	0 100 100	28, 28, 28, 38	0
1	C	2/16 (12%)	0.70	0 100 100	34, 34, 34, 45	0
1	D	2/16 (12%)	-0.10	0 100 100	30, 30, 30, 41	0
1	E	2/16 (12%)	0.09	0 100 100	37, 37, 37, 40	0
1	F	2/16 (12%)	-0.10	0 100 100	43, 43, 43, 44	0
All	All	12/96 (12%)	0.07	0 100 100	28, 37, 44, 45	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	ORD	E	9	8/9	0.91	0.21	-	31,49,70,70	0
1	DVA	B	3	7/8	0.93	0.18	-	18,26,42,42	0
1	DTH	F	15	7/8	0.97	0.12	-	39,48,60,73	0
1	DVA	E	16	7/8	0.67	0.34	-	64,92,106,117	0
1	DAL	D	14	5/6	0.92	0.14	-	38,46,53,55	0
1	DSN	B	8	6/7	0.91	0.19	-	38,46,77,92	0
1	DAL	F	2	5/6	0.95	0.13	-	37,43,49,49	0
1	MV9	E	13	8/9	0.93	0.12	-	30,47,61,63	0
1	DVA	D	6	7/8	0.97	0.12	-	28,45,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DAL	C	14	5/6	0.97	0.13	-	22,33,39,39	0
1	DLE	B	4	8/9	0.96	0.18	-	19,26,42,42	0
1	DAL	C	2	5/6	0.98	0.15	-	18,28,40,40	0
1	ORD	D	1	8/9	0.88	0.30	-	89,113,125,125	0
1	ORD	B	1	8/9	0.93	0.17	-	19,26,31,31	0
1	MV9	B	13	8/9	0.91	0.13	-	22,37,49,49	0
1	DVA	E	10	7/8	0.90	0.16	-	27,46,54,54	0
1	IOY	A	5	12/13	0.90	0.15	-	31,48,80,84	0
1	DVA	D	3	7/8	0.90	0.17	-	52,73,108,108	0
1	ORD	C	1	8/9	0.95	0.15	-	18,33,47,47	0
1	DTH	D	15	7/8	0.91	0.13	-	59,76,87,94	0
1	DVA	F	3	7/8	0.96	0.11	-	32,43,64,64	0
1	DVA	E	3	7/8	0.91	0.18	-	29,55,69,69	0
1	DVA	A	16	7/8	0.85	0.33	-	63,85,98,103	0
1	DVA	C	3	7/8	0.94	0.19	-	22,35,39,42	0
1	DHI	F	11	10/11	0.94	0.10	-	29,38,61,61	0
1	DVA	D	10	7/8	0.93	0.11	-	27,41,45,54	0
1	IOY	F	5	12/13	0.78	0.23	-	31,49,101,168	0
1	ORD	A	9	8/9	0.83	0.19	-	39,49,68,68	0
1	DAL	B	2	5/6	0.97	0.17	-	18,26,34,34	0
1	DAL	B	14	5/6	0.94	0.15	-	25,36,39,43	0
1	DLE	A	4	8/9	0.96	0.10	-	32,46,68,68	0
1	ORD	F	9	8/9	0.93	0.24	-	33,60,73,73	0
1	DLE	E	4	8/9	0.93	0.14	-	32,51,56,66	0
1	DLE	F	4	8/9	0.92	0.15	-	27,55,68,68	0
1	DLE	D	4	8/9	0.93	0.12	-	35,54,84,84	0
1	DAL	F	14	5/6	0.95	0.11	-	36,46,49,55	0
1	DAL	E	14	5/6	0.89	0.17	-	38,49,65,69	0
1	DAL	A	2	5/6	0.92	0.15	-	62,78,93,93	0
1	DLE	C	4	8/9	0.95	0.20	-	22,28,42,42	0
1	IOY	E	5	12/13	0.78	0.25	-	24,44,105,162	0
1	DSN	E	8	6/7	0.90	0.14	-	38,59,80,96	0
1	ORD	E	1	8/9	0.93	0.33	-	39,54,84,84	0
1	DTH	E	15	7/8	0.70	0.29	-	47,77,87,93	0
1	DSN	D	8	6/7	0.84	0.24	-	40,51,65,79	0
1	DVA	C	10	7/8	0.96	0.17	-	40,58,72,72	0
1	MV9	C	13	8/9	0.90	0.15	-	27,42,71,71	0
1	ORD	C	9	8/9	0.81	0.22	-	54,70,82,82	0
1	IOY	D	5	12/13	0.87	0.14	-	30,47,89,111	0
1	DHI	C	11	10/11	0.95	0.16	-	33,47,57,64	0
1	DTH	C	15	7/8	0.95	0.14	-	25,34,46,55	0
1	DVA	B	10	7/8	0.90	0.11	-	30,39,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MV9	D	13	8/9	0.89	0.13	-	32,43,53,53	0
1	DHI	B	11	10/11	0.95	0.13	-	27,36,55,55	0
1	DVA	A	6	7/8	0.97	0.13	-	29,46,72,72	0
1	DHI	A	11	10/11	0.91	0.14	-	31,38,52,63	0
1	DHI	D	11	10/11	0.95	0.12	-	28,34,63,66	0
1	IOY	C	5	12/13	0.90	0.17	-	27,40,71,72	0
1	DSN	A	8	6/7	0.91	0.33	-	41,65,82,99	0
1	DTH	A	15	7/8	0.86	0.12	-	42,60,67,81	0
1	ORD	D	9	8/9	0.91	0.12	-	31,46,60,60	0
1	DAL	A	14	5/6	0.94	0.10	-	36,44,46,48	0
1	DSN	C	8	6/7	0.84	0.17	-	50,72,88,101	0
1	DVA	A	3	7/8	0.82	0.16	-	48,62,81,84	0
1	ORD	B	9	8/9	0.92	0.14	-	40,53,57,63	0
1	ORD	F	1	8/9	0.91	0.21	-	36,55,91,91	0
1	DSN	F	8	6/7	0.93	0.24	-	58,70,93,111	0
1	DVA	B	6	7/8	0.96	0.11	-	24,30,41,41	0
1	DVA	C	16	7/8	0.97	0.14	-	19,29,40,40	0
1	DHI	E	11	10/11	0.96	0.12	-	29,34,47,49	0
1	DVA	F	6	7/8	0.84	0.15	-	35,59,73,73	0
1	DAL	D	2	5/6	0.84	0.15	-	65,88,94,107	0
1	DAL	E	2	5/6	0.88	0.13	-	40,48,53,62	0
1	DVA	D	16	7/8	0.79	0.35	-	74,93,120,120	0
1	MV9	A	13	8/9	0.92	0.13	-	29,39,48,48	0
1	ORD	A	1	8/9	0.88	0.21	-	60,94,117,117	0
1	DVA	E	6	7/8	0.97	0.12	-	24,39,45,47	0
1	DTH	B	15	7/8	0.93	0.15	-	23,34,41,48	0
1	DVA	C	6	7/8	0.96	0.13	-	26,37,53,53	0
1	IOY	B	5	12/13	0.90	0.16	-	23,38,66,68	0
1	DVA	F	16	7/8	0.94	0.11	-	47,62,68,68	0
1	DVA	A	10	7/8	0.94	0.11	-	32,44,49,53	0
1	MV9	F	13	8/9	0.94	0.12	-	37,58,81,81	0
1	DVA	B	16	7/8	0.97	0.11	-	20,27,34,34	0
1	DVA	F	10	7/8	0.95	0.14	-	35,55,58,69	0

## 6.3 Carbohydrates

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( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	101	5/5	0.92	0.17	-	84,84,84,85	5
3	MPD	B	102	8/8	0.60	0.30	-	79,95,96,97	0
3	MPD	C	101	8/8	0.51	0.42	-	68,82,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.