



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:59 AM UTC

PDB ID : 1APV / pdb_00001apv
Title : CRYSTALLOGRAPHIC ANALYSIS OF TRANSITION STATE MIMICS
BOUND TO PENICILLOPEPSIN: DIFLUOROSTATINE-AND DIFLUOR
OSTATONE-CONTAINING PEPTIDES
Authors : Sielecki, A.R.; James, M.N.G.
Deposited on : 1991-12-16
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

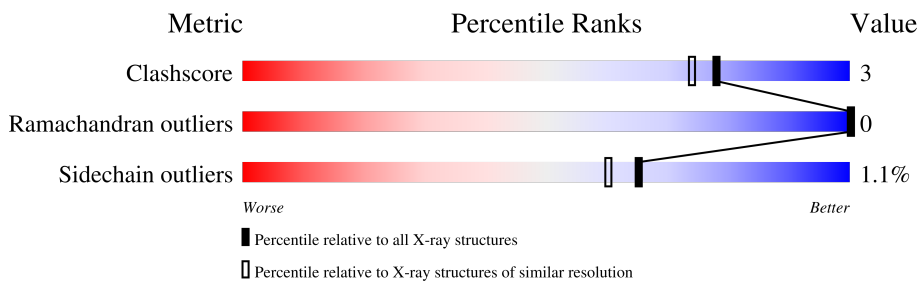
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	323	
2	I	5	

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
4	XYS	E	399	X	-	-	-
5	SO4	E	365	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2709 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.

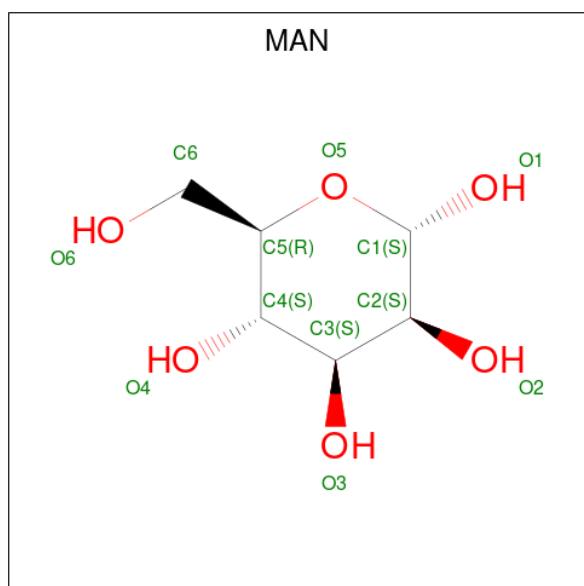
- Molecule 1 is a protein called PENICILLOPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	323	Total	C	N	O	S	0	0	0
			2366	1479	377	508	2			

- Molecule 2 is a protein called INHIBITOR ISOVALERYL (IVA)-VAL-VAL-HYDRATED DIFLUOROSTATONE-N-METHYLAMINE.

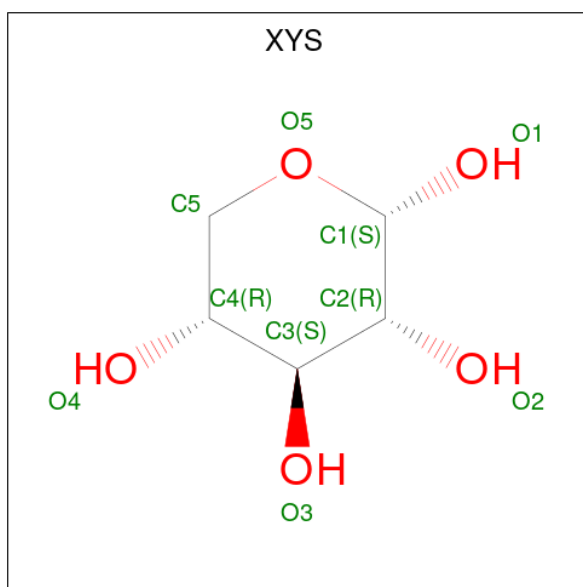
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	5	Total	C	F	N	O	0	0	1
			36	24	2	4	6			

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



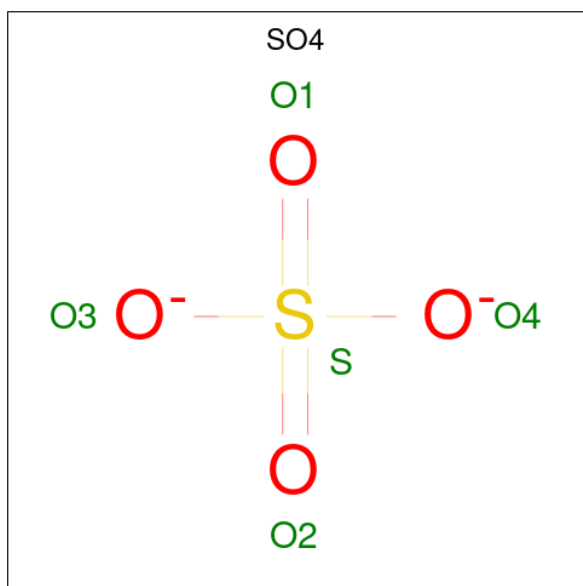
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is alpha-D-xylopyranose (CCD ID: XYS) (formula: C₅H₁₀O₅).



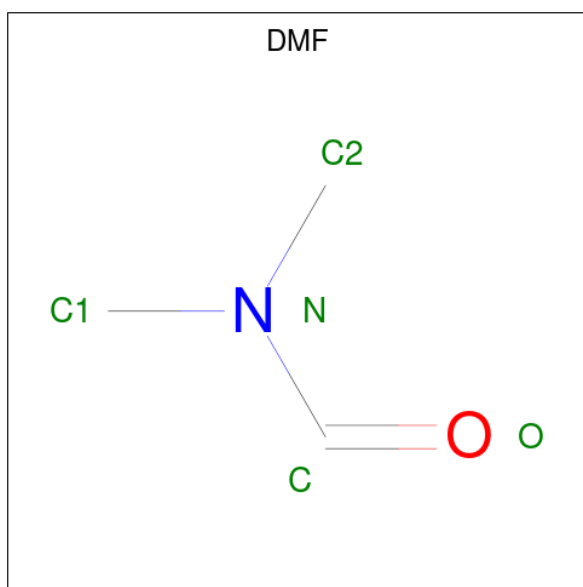
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			9	5	4		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C₃H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	I	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	274	Total	O	0	0
			274	274		
7	I	3	Total	O	0	0
			3	3		

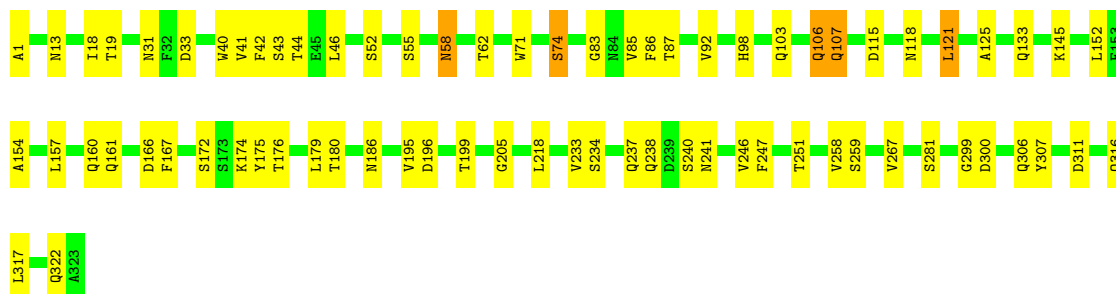
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

• Molecule 1: PENICILLOPEPSIN

Chain E: 



• Molecule 2: INHIBITOR ISOVALERYL (IVA)-VAL-VAL-HYDRATED DIFLUOROSTATON E-N-METHYLAMINE

Chain I: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.52Å 46.57Å 66.23Å 90.00° 116.03° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.131 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2709	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, XYS, SO4, DFO, IVA, DMF, NME

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	E	1.40	4/2420 (0.2%)	2.03	62/3304 (1.9%)
2	I	1.24	0/13	2.12	0/17
All	All	1.40	4/2433 (0.2%)	2.03	62/3321 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	205	GLY	N-CA	6.20	1.51	1.45
1	E	176	THR	CA-CB	5.42	1.61	1.53
1	E	86	PHE	C-O	5.40	1.30	1.23
1	E	259	SER	N-CA	5.39	1.52	1.46

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	281	SER	N-CA-C	9.49	125.26	111.87
1	E	83	GLY	O-C-N	8.98	131.26	123.80
1	E	55	SER	N-CA-C	-8.06	96.09	109.24
1	E	247	PHE	CA-CB-CG	-7.78	106.02	113.80
1	E	167	PHE	CA-CB-CG	-7.70	106.10	113.80
1	E	307	TYR	N-CA-C	-7.63	96.79	109.07
1	E	160	GLN	CG-CD-NE2	7.49	127.63	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	ASP	N-CA-CB	-7.26	99.81	110.84
1	E	52	SER	O-C-N	7.12	131.69	122.93
1	E	133	GLN	OE1-CD-NE2	7.12	129.72	122.60
1	E	98	HIS	CA-CB-CG	-7.12	106.68	113.80
1	E	13	ASN	OD1-CG-ND2	6.59	129.19	122.60
1	E	58	ASN	CB-CA-C	6.59	118.90	110.34
1	E	238	GLN	OE1-CD-NE2	6.57	129.16	122.60
1	E	258	VAL	O-C-N	6.41	129.86	123.00
1	E	160	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	E	199	THR	CA-CB-OG1	-6.29	100.17	109.60
1	E	62	THR	N-CA-CB	-6.26	101.11	111.06
1	E	316	GLN	O-C-N	6.22	129.79	123.26
1	E	115	ASP	CA-C-O	-6.15	114.52	120.92
1	E	195	VAL	N-CA-CB	6.10	122.00	111.39
1	E	267	VAL	N-CA-C	-6.09	101.09	107.60
1	E	241	ASN	OD1-CG-ND2	5.94	128.54	122.60
1	E	174	LYS	CG-CD-CE	5.92	124.91	111.30
1	E	125	ALA	N-CA-C	-5.85	102.28	110.35
1	E	186	ASN	O-C-N	5.84	129.53	122.35
1	E	85	VAL	N-CA-C	5.82	117.07	108.45
1	E	43	SER	O-C-N	5.75	130.43	122.78
1	E	237	GLN	O-C-N	5.64	129.70	123.33
1	E	166	ASP	CA-C-N	-5.62	115.24	123.00
1	E	166	ASP	C-N-CA	-5.62	115.24	123.00
1	E	317	LEU	CA-C-O	-5.61	114.64	120.70
1	E	86	PHE	CA-CB-CG	-5.61	108.19	113.80
1	E	196	ASP	CA-CB-CG	-5.59	107.00	112.60
1	E	234	SER	O-C-N	5.56	129.84	122.95
1	E	92	VAL	O-C-N	5.53	128.93	123.18
1	E	154	ALA	O-C-N	5.49	129.81	123.17
1	E	118	ASN	O-C-N	5.41	130.19	123.15
1	E	311	ASP	N-CA-CB	-5.41	102.06	110.55
1	E	240	SER	CA-C-O	-5.39	114.00	120.10
1	E	41	VAL	O-C-N	5.39	129.11	123.02
1	E	161	GLN	N-CA-CB	5.38	120.32	111.17
1	E	106	GLN	N-CA-C	-5.36	107.28	113.88
1	E	218	LEU	O-C-N	5.33	129.79	122.59
1	E	180	THR	CA-C-O	-5.33	114.58	120.38
1	E	246	VAL	O-C-N	5.29	128.91	123.04
1	E	1	ALA	CB-CA-C	5.24	118.36	110.50
1	E	19	THR	O-C-N	5.24	127.44	121.94
1	E	121	LEU	N-CA-CB	-5.22	102.16	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	87	THR	N-CA-C	-5.21	101.67	109.95
1	E	46	LEU	O-C-N	5.20	128.10	121.34
1	E	157	LEU	CA-C-O	-5.19	115.04	120.80
1	E	42	PHE	N-CA-C	-5.17	102.73	110.23
1	E	317	LEU	O-C-N	5.14	129.91	123.23
1	E	145	LYS	N-CA-C	5.11	117.52	111.33
1	E	299	GLY	CA-C-O	5.10	127.98	122.47
1	E	307	TYR	CA-C-N	-5.09	116.47	123.14
1	E	307	TYR	C-N-CA	-5.09	116.47	123.14
1	E	300	ASP	O-C-N	5.09	127.51	122.12
1	E	74	SER	CB-CA-C	5.08	118.90	109.70
1	E	299	GLY	O-C-N	-5.08	118.44	122.81
1	E	281	SER	N-CA-CB	-5.01	103.57	111.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	1	DFO	Mainchain

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	E	2366	0	2181	13	0
2	I	36	0	39	1	0
3	E	11	0	10	0	0
4	E	9	0	8	0	0
5	E	5	0	0	2	0
6	I	5	0	7	0	0
7	E	274	0	0	0	0
7	I	3	0	0	0	0
All	All	2709	0	2245	13	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 (13) 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:E:106:GLN:C	1:E:107:GLN:HG2	2.06	0.80
1:E:233:VAL:HG13	1:E:251:THR:HG21	1.89	0.55
1:E:121:LEU:HD21	2:I:1:DFO:HD12	1.90	0.54
1:E:179:LEU:N	5:E:365:SO4:O2	2.35	0.54
1:E:306:GLN:C	1:E:322:GLN:HG3	2.39	0.48
1:E:107:GLN:HE21	1:E:107:GLN:HB3	1.54	0.44
1:E:172:SER:HA	1:E:175:TYR:CE1	2.54	0.43
1:E:40:TRP:HA	1:E:103:GLN:O	2.19	0.43
1:E:71:TRP:CE2	1:E:103:GLN:HB3	2.54	0.42
1:E:31:ASN:C	1:E:31:ASN:HD22	2.29	0.41
1:E:44:THR:HG21	1:E:58:ASN:HB2	2.04	0.40
1:E:175:TYR:OH	5:E:365:SO4:O4	2.22	0.40
1:E:152:LEU:HD12	1:E:152:LEU:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	E	321/323 (99%)	319 (99%)	2 (1%)	0	100	100
2	I	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	323/328 (98%)	320 (99%)	3 (1%)	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	E	259/259 (100%)	256 (99%)	3 (1%)	63	57
2	I	2/2 (100%)	2 (100%)	0	100	100
All	All	261/261 (100%)	258 (99%)	3 (1%)	65	60

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	18	ILE
1	E	74	SER
1	E	107	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	13	ASN
1	E	31	ASN
1	E	107	GLN
1	E	306	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	DFO	I	1	2	11,13,14	2.34	1 (9%)	8,20,22	0.67	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	DFO	I	1	2	-	0/8/22/25	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	DFO	OH2-CH	7.23	1.47	1.40

There are no bond angle outliers.

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
2	I	1	DFO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
5	SO4	E	365	-	4,4,4	0.62	0	6,6,6	0.31	0
4	XYS	E	399	1	9,9,10	1.14	0	10,12,14	3.26	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	328	1	11,11,12	0.99	0	15,15,17	1.15	2 (13%)
6	DMF	I	587	-	4,4,4	0.36	0	4,4,4	0.66	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
6	DMF	I	587	-	-	1/2/2/2	-
4	XYS	E	399	1	4/4/3/4	-	0/1/1/1
3	MAN	E	328	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	399	XYS	C5-O5-C1	6.83	122.44	111.42
4	E	399	XYS	C5-C4-C3	5.84	118.14	109.64
4	E	399	XYS	O4-C4-C5	3.72	117.74	109.22
3	E	328	MAN	O2-C2-C1	-2.78	102.86	109.22
4	E	399	XYS	O2-C2-C3	2.61	115.55	110.15
3	E	328	MAN	C3-C4-C5	-2.09	106.44	110.23

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	399	XYS	C3
4	E	399	XYS	C1
4	E	399	XYS	C4
4	E	399	XYS	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	587	DMF	O-C-N-C1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	365	SO4	2	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.