



# wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 02:47 AM GMT

PDB ID : 2AJC  
Title : Porcine dipeptidyl peptidase IV (CD26) in complex with 4-(2-Aminoethyl)-benzenesulphonyl fluoride (AEBSF)  
Authors : Engel, M.; Hoffmann, T.; Manhart, S.; Heiser, U.; Chambre, S.; Huber, R.; Demuth, H.U.; Bode, W.  
Deposited on : 2005-08-01  
Resolution : 1.95 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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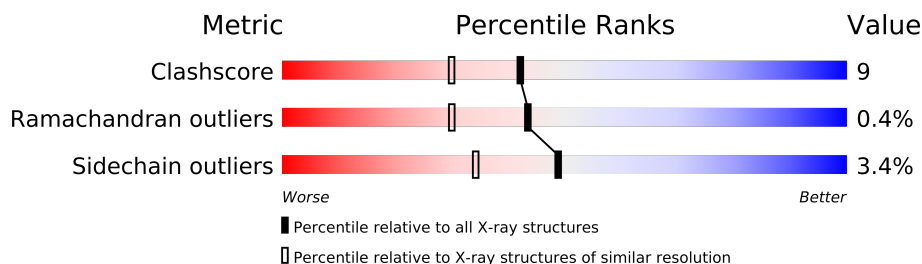
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.95 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	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	728	
1	B	728	
1	C	728	
1	D	728	

## 2 Entry composition i

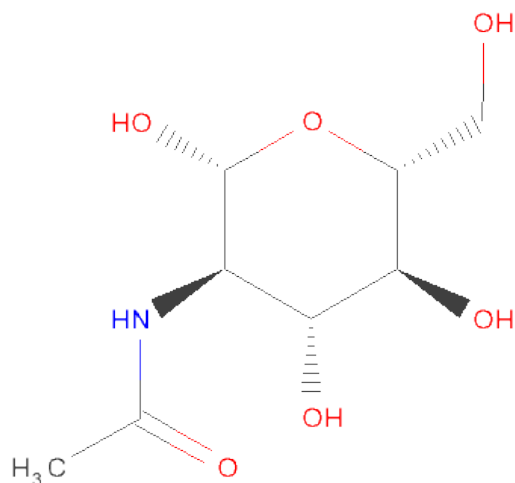
There are 7 unique types of molecules in this entry. The entry contains 25912 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	80	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	42	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	79	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	36	0	0
			5966	3825	986	1132	23			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	3	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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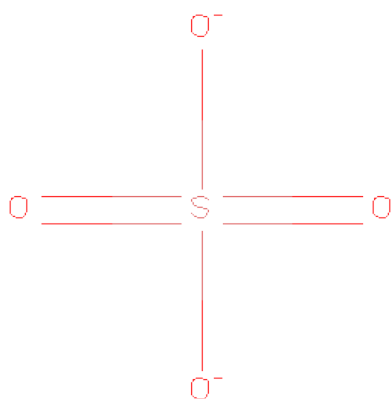
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

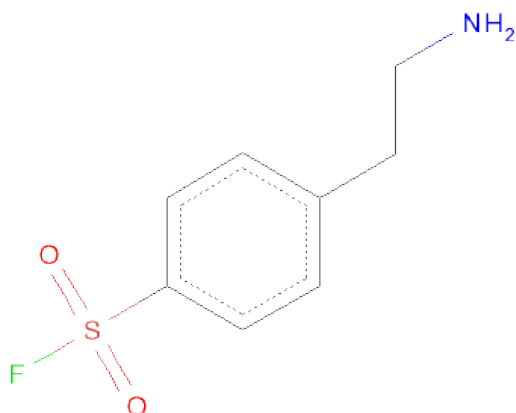
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 6 is 4-(2-AMINOETHYL)BENZENESULFONYLFLUORIDE (three-letter code: AES) (formula: C<sub>8</sub>H<sub>10</sub>FNO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
6	B	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
6	C	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
6	D	1	Total	C	N	O	S	0	0
			12	8	1	2	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	354	Total	O	0	0
			354	354		
7	B	433	Total	O	0	0
			433	433		
7	C	385	Total	O	0	0
			385	385		
7	D	324	Total	O	0	0
			324	324		

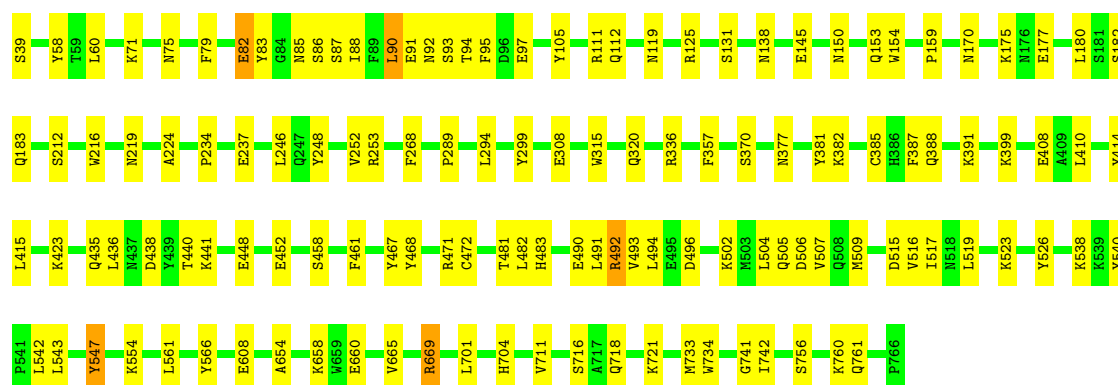
### 3 Residue-property plots

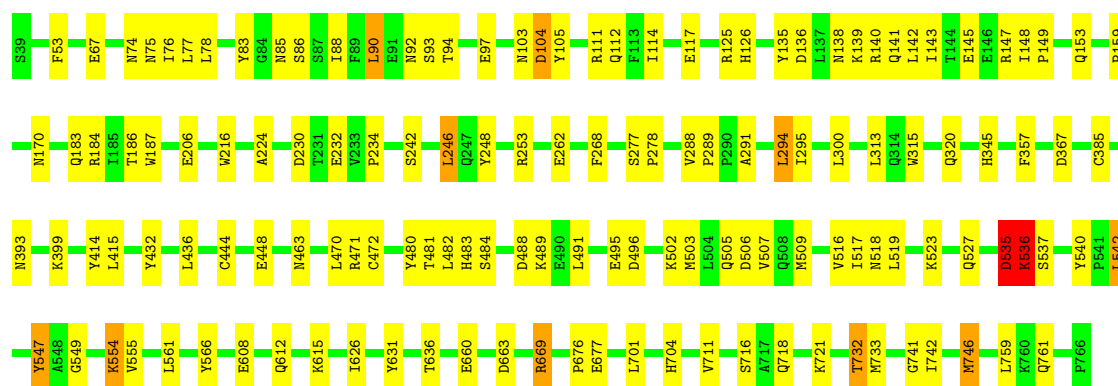
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS failed to run properly.

- Molecule 1: Dipeptidyl peptidase 4

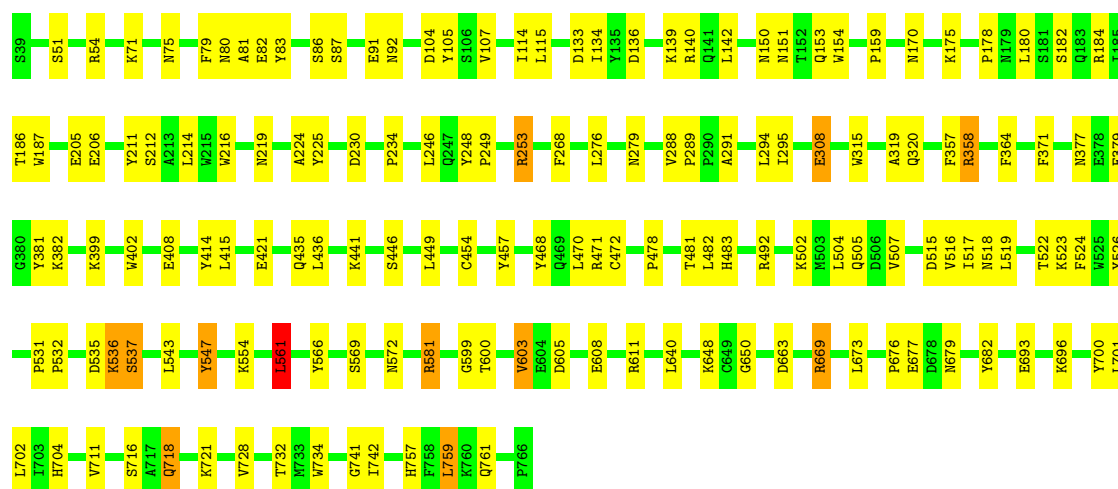
Chain A: 





• Molecule 1: Dipeptidyl peptidase 4

Chain D:





## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.35Å 118.68Å 133.68Å 112.76° 95.16° 90.95°	Depositor
Resolution (Å)	39.90 – 1.95	Depositor
% Data completeness (in resolution range)	96.6 (39.90-1.95)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.234	Depositor
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.362	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 247604 reflections	Xtriage
Total number of atoms	25912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AES, BMA, NAG, 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	0.58	0/6141	0.73	1/8353 (0.0%)
1	B	0.62	0/6141	0.77	3/8353 (0.0%)
1	C	0.60	0/6141	0.76	4/8353 (0.0%)
1	D	0.55	0/6141	0.72	4/8353 (0.0%)
All	All	0.59	0/24564	0.75	12/33412 (0.0%)

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
1	B	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	669	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	B	669	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	C	669	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	D	669	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	D	669	ARG	NE-CZ-NH1	6.45	123.53	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	TYR	Sidechain
1	B	700	TYR	Sidechain
1	D	211	TYR	Sidechain
1	D	700	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5966	0	5662	90	0
1	B	5966	0	5662	103	0
1	C	5966	0	5661	128	0
1	D	5966	0	5662	114	0
2	A	56	0	52	1	0
2	B	56	0	52	1	0
2	C	70	0	65	3	0
2	D	28	0	26	2	0
3	A	56	0	50	0	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	D	84	0	75	1	0
4	B	39	0	34	0	0
4	D	39	0	34	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	12	0	10	1	0
6	B	12	0	10	1	0
6	C	12	0	10	2	0
6	D	12	0	10	2	0
7	A	354	0	0	4	0
7	B	433	0	0	7	0
7	C	385	0	0	7	0
7	D	324	0	0	5	0
All	All	25912	0	23125	421	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 421 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:536:LYS:HG2	1:C:537:SER:H	1.19	1.00
1:C:516:VAL:HG11	1:C:523:LYS:HB2	1.42	0.98
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.71	0.89
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.72	0.88
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.37	0.88

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	A	726/728 (100%)	690 (95%)	33 (4%)	3 (0%)	43	30
1	B	726/728 (100%)	703 (97%)	22 (3%)	1 (0%)	59	51
1	C	726/728 (100%)	692 (95%)	28 (4%)	6 (1%)	27	12
1	D	726/728 (100%)	693 (96%)	32 (4%)	1 (0%)	59	51
All	All	2904/2912 (100%)	2778 (96%)	115 (4%)	11 (0%)	43	30

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ARG
1	C	74	ASN
1	C	103	ASN
1	C	104	ASP
1	C	535	ASP

### 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	652/652 (100%)	633 (97%)	19 (3%)	55	41
1	B	652/652 (100%)	629 (96%)	23 (4%)	48	32
1	C	652/652 (100%)	628 (96%)	24 (4%)	45	30
1	D	652/652 (100%)	630 (97%)	22 (3%)	49	34
All	All	2608/2608 (100%)	2520 (97%)	88 (3%)	49	34

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	701	LEU
1	C	385	CYS
1	D	608	GLU
1	B	702	LEU
1	C	147	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	572	ASN
1	C	75	ASN
1	D	572	ASN
1	B	586	GLN
1	B	704	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

20 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	A	769(A)	1,3	12,14,15	0.64	0	15,19,21	0.75	1 (6%)
3	NAG	A	770(B)	3	12,14,15	0.49	0	15,19,21	0.76	1 (6%)
3	NAG	A	773(A)	1,3	12,14,15	0.67	0	15,19,21	0.94	0
3	NAG	A	774(B)	3	12,14,15	0.51	0	15,19,21	0.76	0
4	NAG	B	768(A)	1,4	12,14,15	0.58	0	15,19,21	0.85	0
4	NAG	B	769(B)	4	12,14,15	0.51	0	15,19,21	0.88	0
4	BMA	B	770(C)	4	10,11,12	0.58	0	11,15,17	1.30	2 (18%)
3	NAG	B	774(A)	1,3	12,14,15	0.60	0	15,19,21	0.90	0
3	NAG	B	775(B)	3	12,14,15	0.52	0	15,19,21	0.89	0
3	NAG	C	772(A)	1,3	12,14,15	0.62	0	15,19,21	0.81	0
3	NAG	C	773(B)	3	12,14,15	0.48	0	15,19,21	0.83	0
4	NAG	D	768(A)	1,4	12,14,15	0.48	0	15,19,21	0.84	0
4	NAG	D	769(B)	4	12,14,15	0.47	0	15,19,21	0.51	0
4	BMA	D	770(C)	4	10,11,12	0.45	0	11,15,17	0.27	0
3	NAG	D	771(A)	1,3	12,14,15	0.56	0	15,19,21	0.76	0
3	NAG	D	772(B)	3	12,14,15	0.48	0	15,19,21	0.68	0
3	NAG	D	774(A)	1,3	12,14,15	0.57	0	15,19,21	0.92	0
3	NAG	D	775(B)	3	12,14,15	0.42	0	15,19,21	0.76	0
3	NAG	D	776(A)	1,3	12,14,15	0.65	0	15,19,21	0.74	0
3	NAG	D	777(B)	3	12,14,15	0.50	0	15,19,21	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
3	NAG	A	769(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	770(B)	3	-	0/6/23/26	0/1/1/1
3	NAG	A	773(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	774(B)	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	768(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	769(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	B	770(C)	4	-	0/2/19/22	0/1/1/1
3	NAG	B	774(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	775(B)	3	-	0/6/23/26	0/1/1/1
3	NAG	C	772(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	773(B)	3	-	0/6/23/26	0/1/1/1
4	NAG	D	768(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	769(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	D	770(C)	4	-	0/2/19/22	0/1/1/1
3	NAG	D	771(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	772(B)	3	-	0/6/23/26	0/1/1/1
3	NAG	D	774(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	775(B)	3	-	0/6/23/26	0/1/1/1
3	NAG	D	776(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	777(B)	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	770(C)	BMA	O5-C5-C6	-2.76	104.08	106.98
3	A	769(A)	NAG	C2-N2-C7	-2.24	119.33	123.09
4	B	770(C)	BMA	C3-C4-C5	2.20	114.14	110.20
3	A	770(B)	NAG	C2-N2-C7	-2.16	119.47	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

23 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	A	1500	-	4,4,4	0.75	0	6,6,6	0.61	0
2	NAG	A	767(A)	1	12,14,15	0.43	0	15,19,21	0.66	0
2	NAG	A	768(A)	1	12,14,15	0.41	0	15,19,21	0.75	0
2	NAG	A	771(A)	1	12,14,15	0.48	0	15,19,21	0.67	0
2	NAG	A	772(A)	1	12,14,15	0.38	0	15,19,21	0.95	0
6	AES	A	801	1	12,12,13	3.97	5 (41%)	14,15,18	1.24	1 (7%)
5	SO4	B	1501	-	4,4,4	0.77	0	6,6,6	0.70	0
2	NAG	B	767(A)	1	12,14,15	0.47	0	15,19,21	0.73	0
2	NAG	B	771(A)	1	12,14,15	0.59	0	15,19,21	0.69	0
2	NAG	B	772(A)	1	12,14,15	0.55	0	15,19,21	1.03	1 (6%)
2	NAG	B	773(A)	1	12,14,15	0.44	0	15,19,21	0.81	0
6	AES	B	801	1	12,12,13	3.53	5 (41%)	14,15,18	1.11	1 (7%)
5	SO4	C	1502	-	4,4,4	0.66	0	6,6,6	0.72	0
2	NAG	C	767(A)	1	12,14,15	0.45	0	15,19,21	1.01	1 (6%)
2	NAG	C	768(A)	1	12,14,15	0.41	0	15,19,21	0.73	0
2	NAG	C	769(A)	1	12,14,15	0.44	0	15,19,21	0.86	0
2	NAG	C	770(A)	1	12,14,15	0.61	0	15,19,21	0.88	1 (6%)
2	NAG	C	771(A)	1	12,14,15	0.44	0	15,19,21	0.88	0
6	AES	C	801	1	12,12,13	4.45	6 (50%)	14,15,18	1.16	1 (7%)
5	SO4	D	1503	-	4,4,4	0.69	0	6,6,6	0.64	0
2	NAG	D	767(A)	1	12,14,15	0.49	0	15,19,21	0.72	0
2	NAG	D	773(A)	1	12,14,15	0.46	0	15,19,21	0.95	1 (6%)
6	AES	D	801	1	12,12,13	4.39	5 (41%)	14,15,18	1.27	1 (7%)

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
5	SO4	A	1500	-	-	0/0/0/0	0/0/0/0
2	NAG	A	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	768(A)	1	-	1/6/23/26	0/1/1/1
2	NAG	A	771(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	772(A)	1	-	0/6/23/26	0/1/1/1
6	AES	A	801	1	-	0/7/7/9	0/1/1/1
5	SO4	B	1501	-	-	0/0/0/0	0/0/0/0
2	NAG	B	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	772(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	773(A)	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AES	B	801	1	-	0/7/7/9	0/1/1/1
5	SO4	C	1502	-	-	0/0/0/0	0/0/0/0
2	NAG	C	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	768(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	769(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	770(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	771(A)	1	-	0/6/23/26	0/1/1/1
6	AES	C	801	1	-	0/7/7/9	0/1/1/1
5	SO4	D	1503	-	-	0/0/0/0	0/0/0/0
2	NAG	D	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	D	773(A)	1	-	1/6/23/26	0/1/1/1
6	AES	D	801	1	-	0/7/7/9	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	801	AES	O2S-S	-12.31	1.46	1.51
6	C	801	AES	O2S-S	-11.88	1.46	1.51
6	A	801	AES	O2S-S	-11.17	1.46	1.51
6	B	801	AES	O2S-S	-9.03	1.47	1.51
6	C	801	AES	O1S-S	-8.11	1.47	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	801	AES	O2S-S-C1	2.95	112.00	104.62
2	C	767(A)	NAG	C3-C2-N2	-2.73	107.60	111.76
6	B	801	AES	O2S-S-C1	2.46	110.78	104.62
6	A	801	AES	O2S-S-C1	2.33	110.46	104.62
2	B	772(A)	NAG	C3-C4-C5	2.33	114.36	110.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	773(A)	NAG	O7-C7-N2-C2
2	A	768(A)	NAG	O7-C7-N2-C2

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.