



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:42 PM GMT

PDB ID : 2AJD
Title : Porcine dipeptidyl peptidase IV (CD26) in complex with L-Pro-boro-L-Pro (boroPro)
Authors : Engel, M.; Hoffmann, T.; Manhart, S.; Heiser, U.; Chambre, S.; Huber, R.; Demuth, H.U.; Bode, W.
Deposited on : 2005-08-01
Resolution : 2.56 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

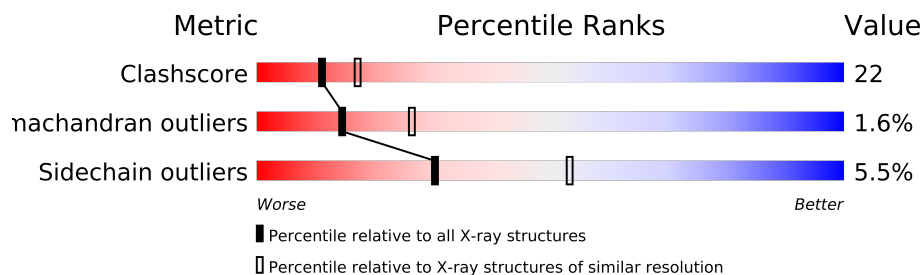
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.56 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	2876 (2.60-2.52)
Ramachandran outliers	78287	2826 (2.60-2.52)
Sidechain outliers	78261	2826 (2.60-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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

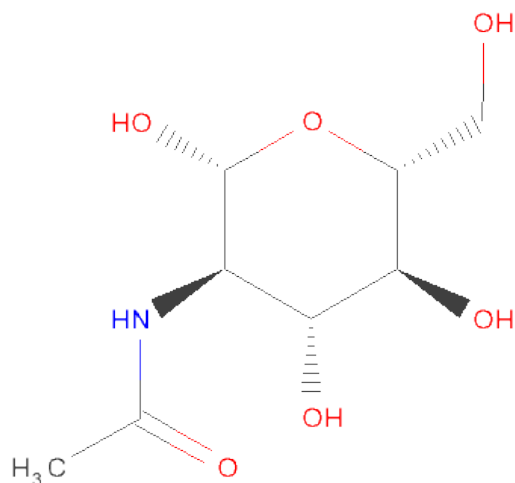
There are 7 unique types of molecules in this entry. The entry contains 25139 atoms, of which 0 are hydrogen and 0 are deuterium.

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	83	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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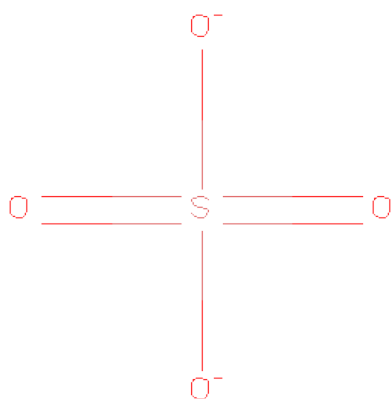
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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

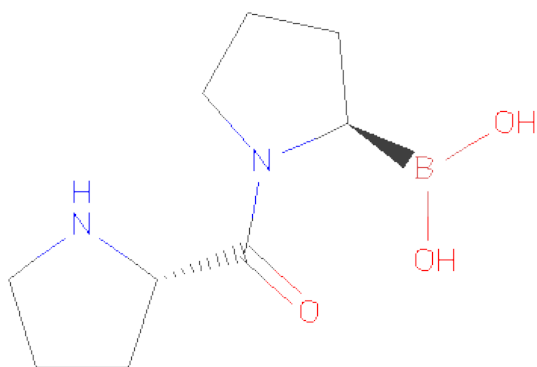
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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 (2R)-N-[(2R)-2-(DIHYDROXYBORYL)-1-L-PROLYLPYRROLIDIN-2-YL]-N-[(5R)-5-(DIHYDROXYBORYL)-1-L-PROLYLPYRROLIDIN-2-YL]-L-PROLINAMIDE (three-letter code: BPR) (formula: C₉H₁₇BN₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	B	C	N	O	0	0
			15	1	9	2	3		
6	B	1	Total	B	C	N	O	0	0
			15	1	9	2	3		
6	C	1	Total	B	C	N	O	0	0
			15	1	9	2	3		
6	D	1	Total	B	C	N	O	0	0
			15	1	9	2	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	163	Total	O	0	0
			163	163		
7	B	224	Total	O	0	0
			224	224		
7	C	138	Total	O	0	0
			138	138		
7	D	186	Total	O	0	0
			186	186		

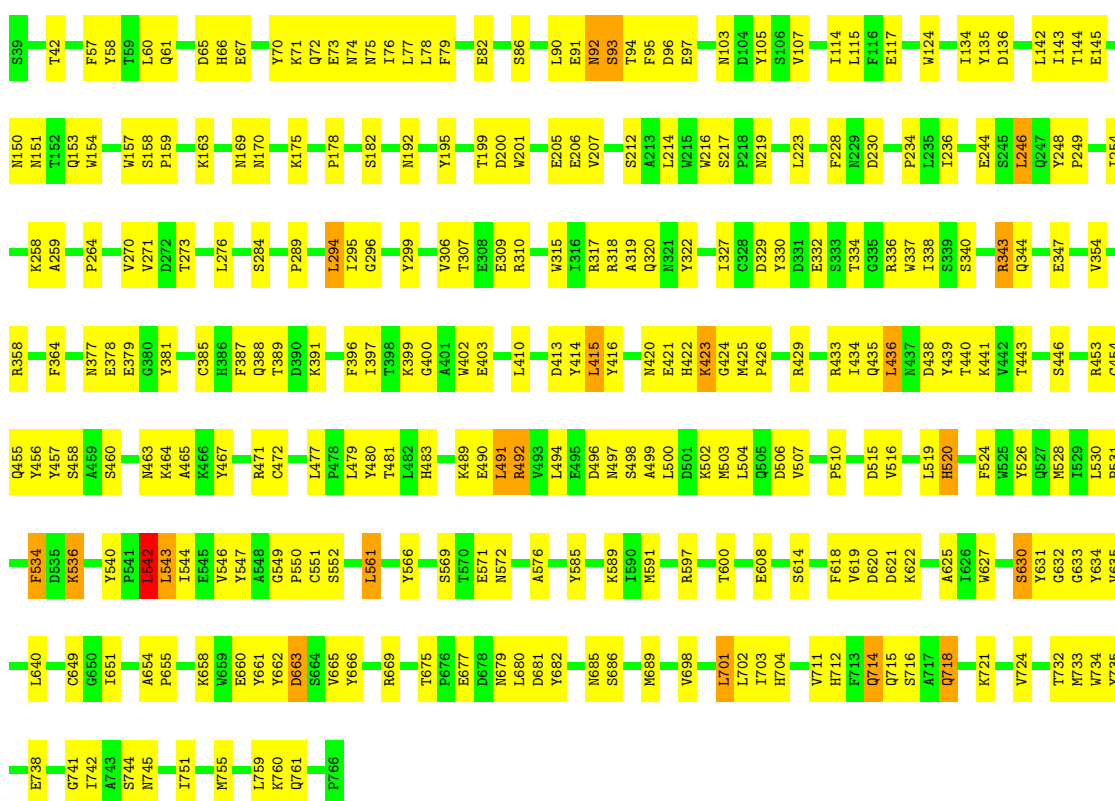
3 Residue-property plots

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 ($RSRZ > 2$). 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.

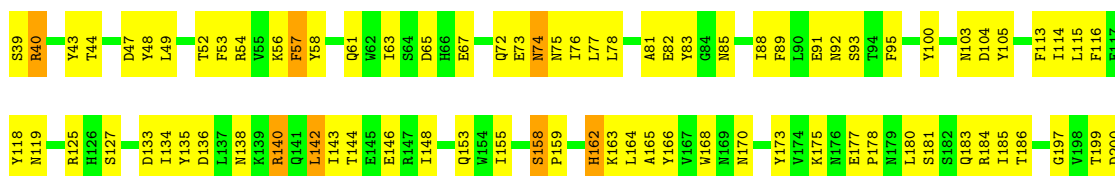
• Molecule 1: Dipeptidyl peptidase 4

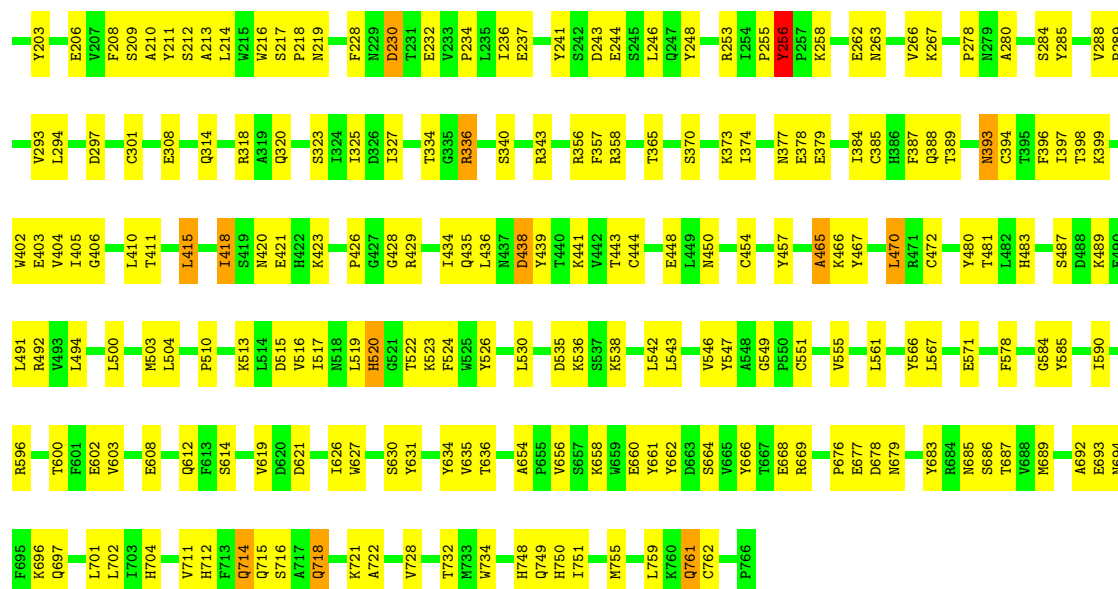
Chain A:



• Molecule 1: Dipeptidyl peptidase 4

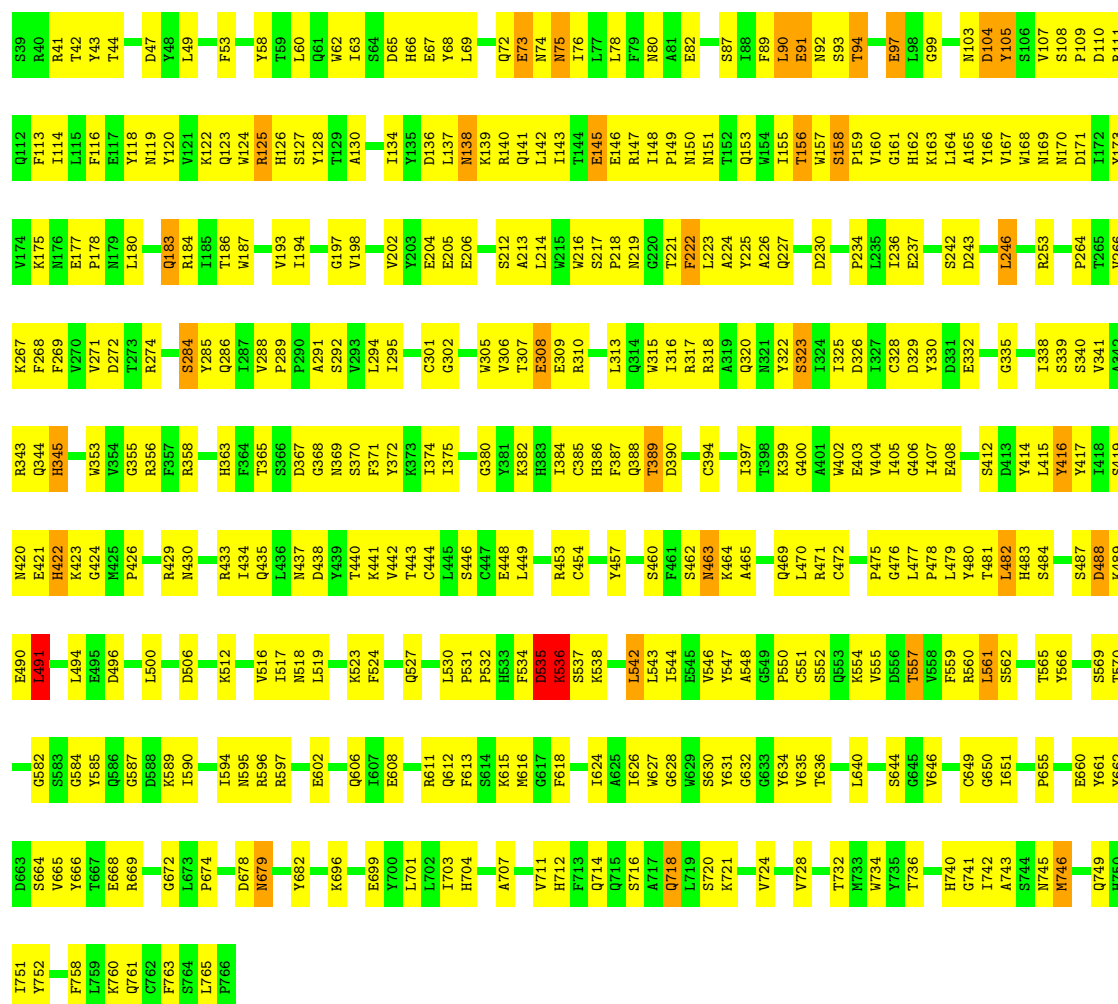
Chain B:





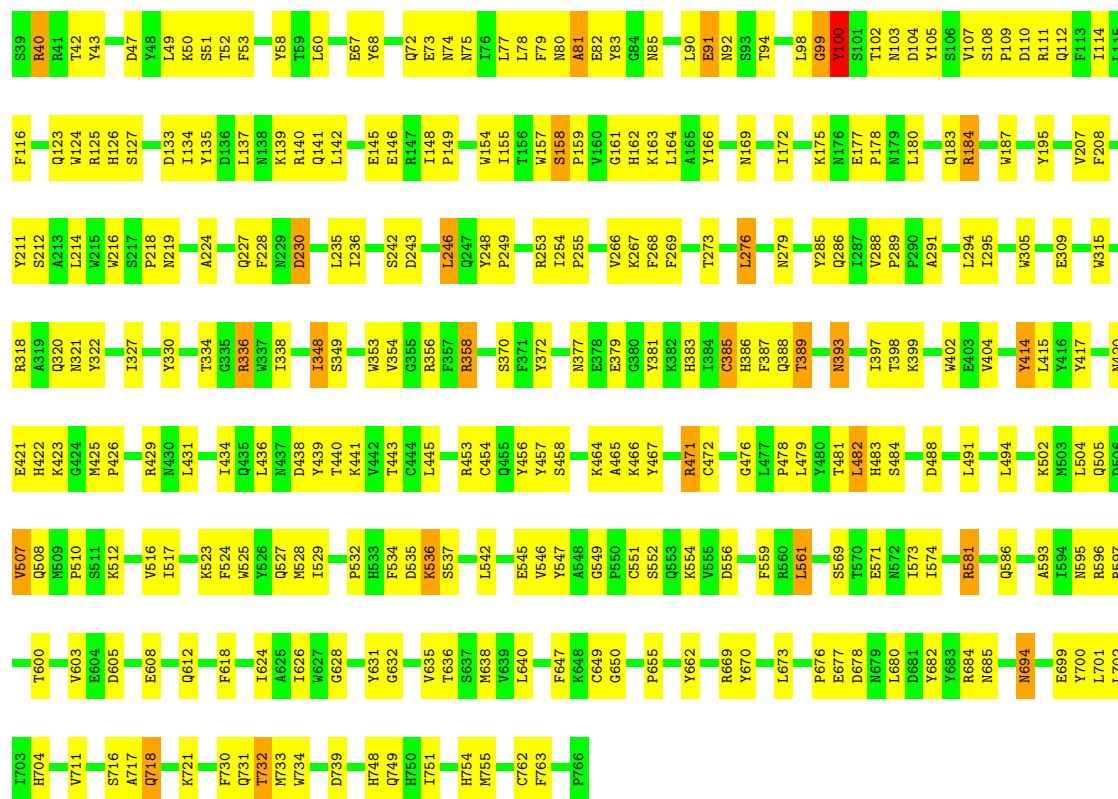
• Molecule 1: Dipeptidyl peptidase 4

Chain C:



● 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, α , β , γ	63.40Å 122.07Å 134.03Å 111.41° 95.27° 94.52°	Depositor
Resolution (Å)	19.99 – 2.56	Depositor
% Data completeness (in resolution range)	96.9 (19.99-2.56)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.312	Depositor
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.637	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 115166 reflections	Xtriage
Total number of atoms	25139	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: BMA, BPR, 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	0.47	0/6141	0.71	1/8353 (0.0%)
1	B	0.50	0/6141	0.73	1/8353 (0.0%)
1	C	0.45	0/6141	0.70	0/8353
1	D	0.49	0/6141	0.73	1/8353 (0.0%)
All	All	0.48	0/24564	0.72	3/33412 (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	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	656	VAL	N-CA-C	-5.96	94.92	111.00
1	A	542	LEU	CA-CB-CG	5.41	127.74	115.30
1	D	529	ILE	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	256	TYR	Sidechain
1	C	285	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	237	0
1	B	5966	0	5662	215	0
1	C	5966	0	5661	359	0
1	D	5966	0	5661	255	0
2	A	56	0	52	1	0
2	B	56	0	52	1	0
2	C	70	0	65	6	0
2	D	28	0	26	1	0
3	A	56	0	50	4	0
3	B	28	0	25	4	0
3	C	28	0	25	2	0
3	D	84	0	75	4	0
4	B	39	0	34	1	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	15	0	17	2	0
6	B	15	0	17	3	0
6	C	15	0	17	4	0
6	D	15	0	17	1	0
7	A	163	0	0	14	0
7	B	224	0	0	14	0
7	C	138	0	0	21	0
7	D	186	0	0	13	0
All	All	25139	0	23152	1057	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 22.

The worst 5 of 1057 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	1.09	1.18
1:D:600:THR:HG22	3:D:776(A):NAG:H83	1.42	1.02
1:B:82:GLU:HG2	1:B:467:TYR:OH	1.65	0.95
1:D:393:ASN:HD22	1:D:393:ASN:H	1.11	0.92
1:A:453:ARG:HH21	1:A:479:LEU:HB2	1.36	0.91

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%)	655 (90%)	60 (8%)	11 (2%)	15	28
1	B	726/728 (100%)	658 (91%)	60 (8%)	8 (1%)	21	39
1	C	726/728 (100%)	610 (84%)	93 (13%)	23 (3%)	6	8
1	D	726/728 (100%)	664 (92%)	58 (8%)	4 (1%)	33	60
All	All	2904/2912 (100%)	2587 (89%)	271 (9%)	46 (2%)	14	26

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	491	LEU
1	B	140	ARG
1	C	91	GLU
1	C	103	ASN

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%)	621 (95%)	31 (5%)	35	60
1	B	652/652 (100%)	610 (94%)	42 (6%)	25	44
1	C	652/652 (100%)	614 (94%)	38 (6%)	28	50
1	D	652/652 (100%)	619 (95%)	33 (5%)	33	57
All	All	2608/2608 (100%)	2464 (94%)	144 (6%)	30	53

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	685	ASN
1	C	183	GLN
1	D	561	LEU
1	B	702	LEU
1	C	75	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	694	ASN
1	C	176	ASN
1	D	612	GLN
1	B	718	GLN
1	C	74	ASN

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	0.50	0	15,19,21	0.77	0
3	NAG	A	770(B)	3	12,14,15	0.52	0	15,19,21	0.82	1 (6%)
3	NAG	A	773(A)	1,3	12,14,15	0.49	0	15,19,21	0.87	0
3	NAG	A	774(B)	3	12,14,15	0.50	0	15,19,21	0.85	1 (6%)
4	NAG	B	768(A)	1,4	12,14,15	0.61	0	15,19,21	0.69	0
4	NAG	B	769(B)	4	12,14,15	0.66	0	15,19,21	0.78	0
4	BMA	B	770(C)	4	10,11,12	0.55	0	11,15,17	0.31	0
3	NAG	B	774(A)	1,3	12,14,15	0.51	0	15,19,21	0.98	1 (6%)
3	NAG	B	775(B)	3	12,14,15	0.46	0	15,19,21	1.00	1 (6%)
3	NAG	C	772(A)	1,3	12,14,15	0.49	0	15,19,21	0.98	0
3	NAG	C	773(B)	3	12,14,15	0.50	0	15,19,21	0.83	1 (6%)
4	NAG	D	768(A)	1,4	12,14,15	0.41	0	15,19,21	0.70	0
4	NAG	D	769(B)	4	12,14,15	0.54	0	15,19,21	0.57	0
4	BMA	D	770(C)	4	10,11,12	0.47	0	11,15,17	0.23	0
3	NAG	D	771(A)	1,3	12,14,15	0.48	0	15,19,21	0.83	0
3	NAG	D	772(B)	3	12,14,15	0.59	0	15,19,21	0.83	1 (6%)
3	NAG	D	774(A)	1,3	12,14,15	0.60	0	15,19,21	1.12	1 (6%)
3	NAG	D	775(B)	3	12,14,15	0.51	0	15,19,21	0.72	0
3	NAG	D	776(A)	1,3	12,14,15	0.48	0	15,19,21	0.81	0
3	NAG	D	777(B)	3	12,14,15	0.57	0	15,19,21	0.84	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	774(A)	NAG	C3-C2-N2	-2.51	107.94	111.76
3	B	775(B)	NAG	C3-C2-N2	-2.40	108.11	111.76
3	C	773(B)	NAG	C3-C2-N2	-2.28	108.28	111.76
3	A	770(B)	NAG	C2-N2-C7	-2.26	119.30	123.09
3	D	772(B)	NAG	C2-N2-C7	-2.22	119.35	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	0.55	0	6,6,6	0.64	0
2	NAG	A	767(A)	1	12,14,15	0.51	0	15,19,21	0.66	0
2	NAG	A	768(A)	1	12,14,15	0.46	0	15,19,21	0.80	1 (6%)
2	NAG	A	771(A)	1	12,14,15	0.60	0	15,19,21	0.62	0
2	NAG	A	772(A)	1	12,14,15	0.41	0	15,19,21	0.81	1 (6%)
6	BPR	A	801	1	16,16,16	0.55	0	22,22,22	1.72	2 (9%)
5	SO4	B	1501	-	4,4,4	0.60	0	6,6,6	0.67	0
2	NAG	B	767(A)	1	12,14,15	0.50	0	15,19,21	0.79	1 (6%)
2	NAG	B	771(A)	1	12,14,15	0.32	0	15,19,21	0.76	0
2	NAG	B	772(A)	1	12,14,15	0.48	0	15,19,21	0.88	1 (6%)
2	NAG	B	773(A)	1	12,14,15	0.55	0	15,19,21	0.96	1 (6%)
6	BPR	B	801	1	16,16,16	1.19	1 (6%)	22,22,22	1.64	3 (13%)
5	SO4	C	1502	-	4,4,4	0.70	0	6,6,6	0.74	0
2	NAG	C	767(A)	1	12,14,15	0.43	0	15,19,21	0.69	0
2	NAG	C	768(A)	1	12,14,15	0.43	0	15,19,21	0.76	0
2	NAG	C	769(A)	1	12,14,15	0.43	0	15,19,21	0.84	0
2	NAG	C	770(A)	1	12,14,15	0.65	0	15,19,21	0.72	0
2	NAG	C	771(A)	1	12,14,15	0.57	0	15,19,21	0.77	0
6	BPR	C	801	1	16,16,16	0.82	0	22,22,22	1.71	3 (13%)
5	SO4	D	1503	-	4,4,4	0.81	0	6,6,6	0.68	0
2	NAG	D	767(A)	1	12,14,15	0.53	0	15,19,21	0.66	0
2	NAG	D	773(A)	1	12,14,15	0.59	0	15,19,21	0.78	0
6	BPR	D	801	1	16,16,16	0.57	0	22,22,22	1.64	3 (13%)

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	-	0/6/23/26	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	BPR	A	801	1	-	0/10/29/29	0/2/2/2
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	BPR	B	801	1	-	0/10/29/29	0/2/2/2
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	-	1/6/23/26	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	BPR	C	801	1	-	0/10/29/29	0/2/2/2
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	-	0/6/23/26	0/1/1/1
6	BPR	D	801	1	-	0/10/29/29	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	801	BPR	B-C2	3.89	1.62	1.57

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	BPR	O1-B-C2	-5.55	109.37	121.13
6	B	801	BPR	O1-B-C2	-5.11	110.31	121.13
6	D	801	BPR	O1-B-C2	-5.07	110.39	121.13
6	C	801	BPR	O1-B-C2	-5.04	110.45	121.13
6	A	801	BPR	O2-B-C2	-4.67	111.25	121.13

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	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.