



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:43 PM GMT

PDB ID : 2AJB
Title : Porcine dipeptidyl peptidase IV (CD26) in complex with the tripeptide tert-butyl-Gly-L-Pro-L-Ile(tBu-GPI)
Authors : Engel, M.; Hoffmann, T.; Manhart, S.; Heiser, U.; Chambre, S.; Huber, R.; Demuth, H.U.; Bode, W.
Deposited on : 2005-08-01
Resolution : 2.75 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>

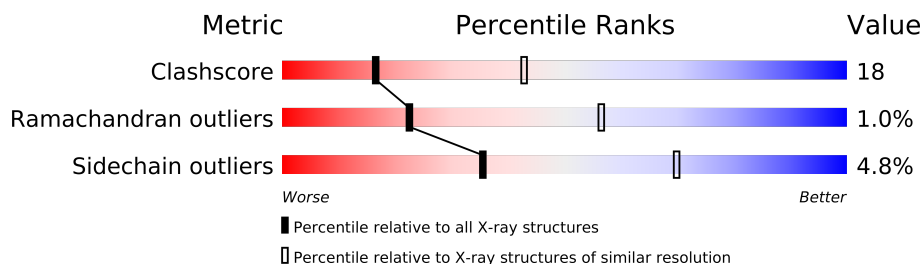
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.75 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	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)

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

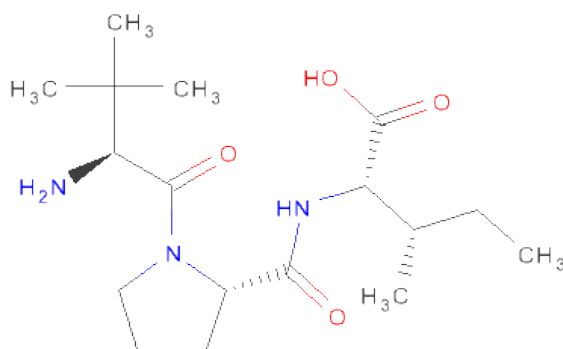
There are 7 unique types of molecules in this entry. The entry contains 25306 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-METHYL-L-VALYL-L-PROLYL-L-ISOLEUCINE (three-letter code: 0QG) (formula: $C_{17}H_{31}N_3O_4$).



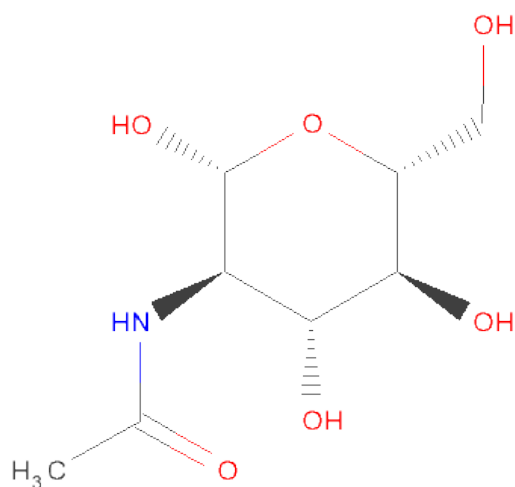
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	9	0
			24	17	3	4		
2	B	1	Total	C	N	O	9	0
			24	17	3	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	9	0
			24	17	3	4		
2	D	1	Total	C	N	O	9	0
			24	17	3	4		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	189	Total	O	0	0
			189	189		
7	B	219	Total	O	0	0
			219	219		
7	C	219	Total	O	0	0
			219	219		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	215	Total 215	O 215	0	0

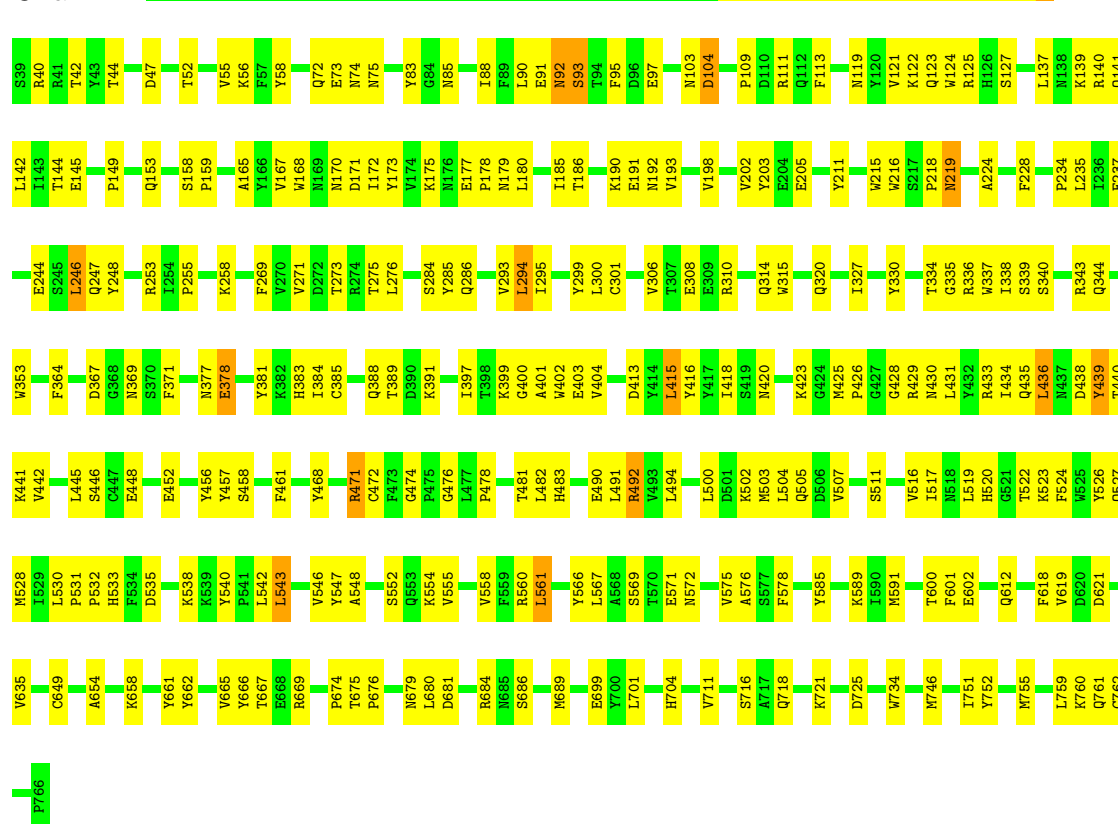
3 Residue-property plots

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.

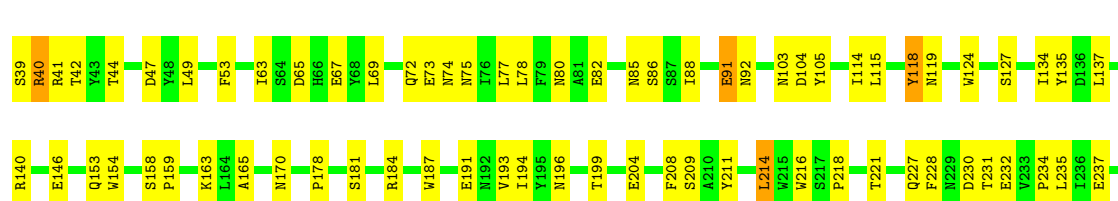
• Molecule 1: Dipeptidyl peptidase 4

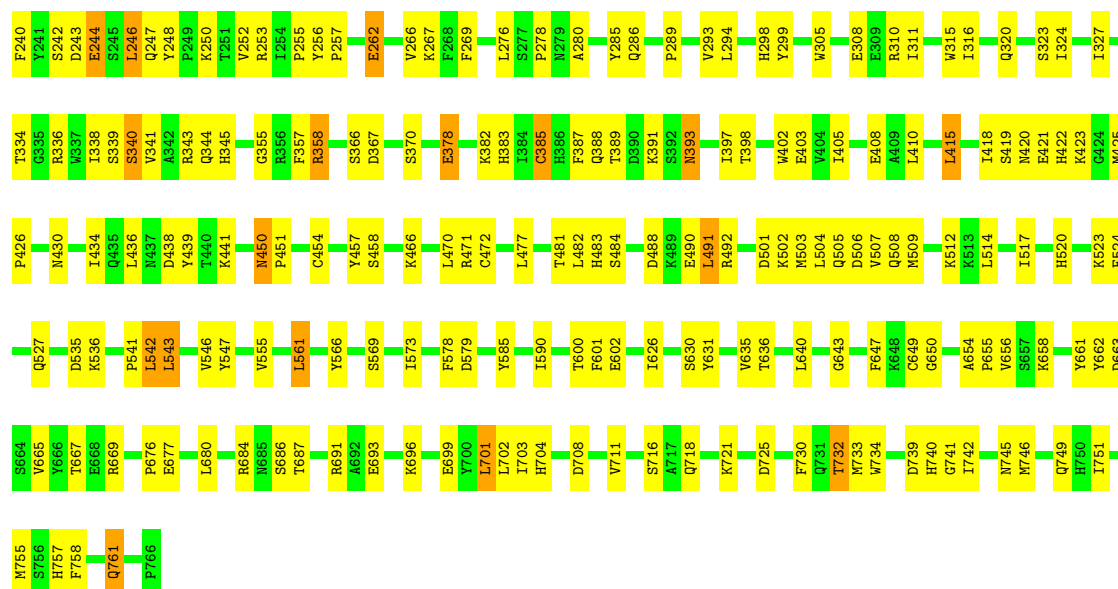
Chain A:



• Molecule 1: Dipeptidyl peptidase 4

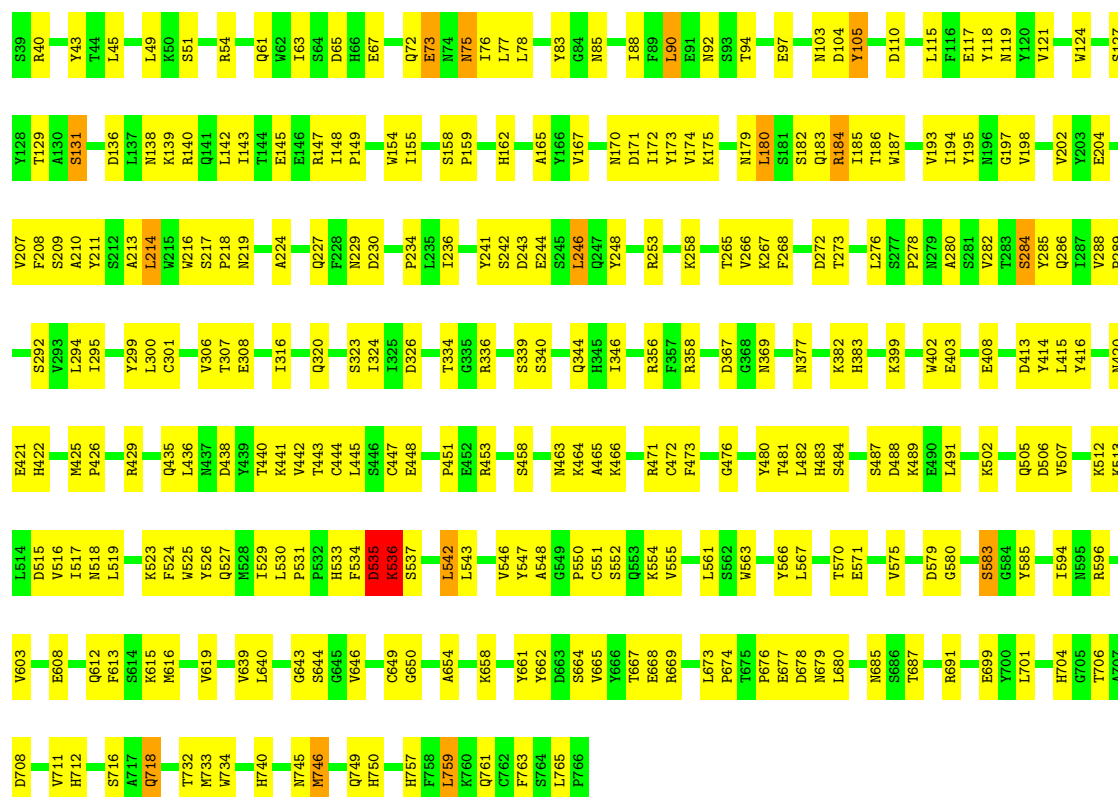
Chain B:





• Molecule 1: Dipeptidyl peptidase 4

Chain C:



• Molecule 1: Dipeptidyl peptidase 4

Chain D:



V728	F618	V516	S419	I324	L235	D133
T732	V619	L519	M420	I325	I236	I134
Y735	D620	H520	E421	D326	E244	Y135
M746	Y631	G521	K423	I327	S245	D136
	L640	T522	P426	Y330	L246	L137
T751	G645	K523	L431	D331	Q247	K139
M755	G650	F524	L436	E332	Y248	R140
S756	G651	H525	N437	G335	R253	Q141
H757	I651	Q527	D438	Q344	L142	I143
F758	A654	L530	Y439	G352	P257	T144
L759	K658	P531	T440	W353	K258	Q153
P766	W659	P532	E448	V354	A259	W154
	E660	D535	Y457	G355	F268	I155
	Y661	K536	S460	R356	F269	P159
	D663	S537	P461	F357	V270	N169
	V665	K539	S462	R358	V271	N170
		L543	N463	P359	D272	Y173
		V546	S464	F364	T273	Y173
		Y547	N464	T365	R274	P178
		G549	A465	S370	T275	P178
		S552	Y468	F371	L276	R184
		Q553	R471	N377	N279	W187
		K554	C472	E378	S284	K190
		V555	F473	E379	Y285	E191
		D556	G474	K382	Q286	E191
		T557	P478	H383	I287	N192
		L561	L482	I384	V288	V193
		A564	H483	C385	P289	N196
		T565	S484	H386	A291	G197
		Y566	S486	F387	S292	V198
		S569	S487	Q388	V293	T199
		V575	D488	T389	L294	F208
		R581	R492	N393	I295	Y211
		G586	L494	D297	G296	S212
		G587	N497	H298	D297	A213
		K588	K502	T398	Y299	L214
		K589	M503	K399	V303	W215
		L590	L504	V402	E308	W216
		M591	Q505	E403	L313	W219
		N595	D506	V404	Q314	L223
		S716	V507	E408	W315	Y225
		A717	P510	A409	I316	Y225
		Q718	S511	L410	R317	F228
			T600	L418	Q320	W229
			F601	I418	N321	D230
					Y322	P234
					S323	

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	62.30Å 118.50Å 133.53Å 112.67° 94.94° 91.02°	Depositor
Resolution (Å)	19.96 – 2.75	Depositor
% Data completeness (in resolution range)	95.8 (19.96-2.75)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.270	Depositor
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.699	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 87140 reflections	Xtriage
Total number of atoms	25306	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, SO4, OQG, NAG

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	0.42	0/6141	0.67	1/8353 (0.0%)
1	B	0.45	0/6141	0.69	1/8353 (0.0%)
1	C	0.44	0/6141	0.69	1/8353 (0.0%)
1	D	0.43	0/6141	0.67	0/8353
All	All	0.44	0/24564	0.68	3/33412 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	LEU	N-CA-C	-5.39	96.45	111.00
1	B	656	VAL	N-CA-C	-5.29	96.72	111.00
1	A	92	ASN	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

There are no planarity outliers.

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	213	0
1	B	5966	0	5662	201	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5966	0	5661	239	0
1	D	5966	0	5661	216	0
2	A	24	0	30	2	0
2	B	24	0	30	0	0
2	C	24	0	30	0	0
2	D	24	0	30	0	0
3	A	56	0	52	0	0
3	B	56	0	52	7	0
3	C	70	0	65	3	0
3	D	28	0	26	1	0
4	A	56	0	50	1	0
4	B	28	0	25	1	0
4	C	28	0	25	2	0
4	D	84	0	75	2	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	B	39	0	34	3	0
6	D	39	0	34	2	0
7	A	189	0	0	11	0
7	B	219	0	0	12	0
7	C	219	0	0	16	0
7	D	215	0	0	16	0
All	All	25306	0	23204	848	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 18.

The worst 5 of 848 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.33	0.93
1:B:393:ASN:H	1:B:393:ASN:HD22	1.12	0.92
6:B:768(A):NAG:H62	6:B:769(B):NAG:H82	1.52	0.91
1:D:75:ASN:ND2	1:D:92:ASN:H	1.71	0.88
1:D:291:ALA:O	1:D:295:ILE:HG13	1.76	0.84

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%)	657 (90%)	61 (8%)	8 (1%)	21	53
1	B	726/728 (100%)	669 (92%)	52 (7%)	5 (1%)	30	67
1	C	726/728 (100%)	649 (89%)	67 (9%)	10 (1%)	16	45
1	D	726/728 (100%)	663 (91%)	57 (8%)	6 (1%)	27	63
All	All	2904/2912 (100%)	2638 (91%)	237 (8%)	29 (1%)	22	56

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	B	40	ARG
1	B	491	LEU
1	C	103	ASN
1	C	105	TYR

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%)	626 (96%)	26 (4%)	42	77
1	B	652/652 (100%)	621 (95%)	31 (5%)	35	70
1	C	652/652 (100%)	617 (95%)	35 (5%)	31	64
1	D	652/652 (100%)	618 (95%)	34 (5%)	32	66
All	All	2608/2608 (100%)	2482 (95%)	126 (5%)	35	70

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	761	GLN
1	C	284	SER
1	D	588	ASP
1	C	75	ASN
1	C	158	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	679	ASN
1	C	176	ASN
1	D	595	ASN
1	B	694	ASN
1	B	761	GLN

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	$\# Z > 2$
4	NAG	A	769(A)	1,4	12,14,15	0.43	0	15,19,21	0.62	0
4	NAG	A	770(B)	4	12,14,15	0.45	0	15,19,21	0.73	0
4	NAG	A	773(A)	1,4	12,14,15	0.46	0	15,19,21	0.85	0
4	NAG	A	774(B)	4	12,14,15	0.46	0	15,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	768(A)	1,6	12,14,15	0.43	0	15,19,21	0.91	1 (6%)
6	NAG	B	769(B)	6	12,14,15	0.48	0	15,19,21	0.80	1 (6%)
6	BMA	B	770(C)	6	10,11,12	0.40	0	11,15,17	0.29	0
4	NAG	B	774(A)	1,4	12,14,15	0.51	0	15,19,21	0.92	0
4	NAG	B	775(B)	4	12,14,15	0.47	0	15,19,21	0.97	1 (6%)
4	NAG	C	772(A)	1,4	12,14,15	0.43	0	15,19,21	0.81	0
4	NAG	C	773(B)	4	12,14,15	0.47	0	15,19,21	0.79	0
6	NAG	D	768(A)	1,6	12,14,15	0.55	0	15,19,21	0.91	0
6	NAG	D	769(B)	6	12,14,15	0.54	0	15,19,21	0.54	0
6	BMA	D	770(C)	6	10,11,12	0.51	0	11,15,17	0.51	0
4	NAG	D	771(A)	1,4	12,14,15	0.53	0	15,19,21	0.73	0
4	NAG	D	772(B)	4	12,14,15	0.50	0	15,19,21	0.74	0
4	NAG	D	774(A)	1,4	12,14,15	0.57	0	15,19,21	1.03	1 (6%)
4	NAG	D	775(B)	4	12,14,15	0.47	0	15,19,21	0.83	0
4	NAG	D	776(A)	1,4	12,14,15	0.50	0	15,19,21	0.65	0
4	NAG	D	777(B)	4	12,14,15	0.50	0	15,19,21	0.86	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
4	NAG	A	769(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	770(B)	4	-	0/6/23/26	0/1/1/1
4	NAG	A	773(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	774(B)	4	-	0/6/23/26	0/1/1/1
6	NAG	B	768(A)	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	769(B)	6	-	0/6/23/26	0/1/1/1
6	BMA	B	770(C)	6	-	0/2/19/22	0/1/1/1
4	NAG	B	774(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	775(B)	4	-	0/6/23/26	0/1/1/1
4	NAG	C	772(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	773(B)	4	-	0/6/23/26	0/1/1/1
6	NAG	D	768(A)	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	769(B)	6	-	1/6/23/26	0/1/1/1
6	BMA	D	770(C)	6	-	0/2/19/22	0/1/1/1
4	NAG	D	771(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	772(B)	4	-	0/6/23/26	0/1/1/1
4	NAG	D	774(A)	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	775(B)	4	-	0/6/23/26	0/1/1/1
4	NAG	D	776(A)	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	777(B)	4	-	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(°)
6	B	768(A)	NAG	C3-C2-N2	-2.53	107.91	111.76
4	B	775(B)	NAG	C3-C2-N2	-2.45	108.03	111.76
4	D	774(A)	NAG	C2-N2-C7	-2.28	119.25	123.09
6	B	769(B)	NAG	C2-N2-C7	-2.10	119.57	123.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	774(A)	NAG	O7-C7-N2-C2
6	D	769(B)	NAG	O7-C7-N2-C2

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	0.60	0	6,6,6	0.58	0
3	NAG	A	767(A)	1	12,14,15	0.44	0	15,19,21	0.72	0
3	NAG	A	768(A)	1	12,14,15	0.46	0	15,19,21	0.72	0
3	NAG	A	771(A)	1	12,14,15	0.48	0	15,19,21	0.64	0
3	NAG	A	772(A)	1	12,14,15	0.43	0	15,19,21	0.86	1 (6%)
2	0QG	A	802	1	24,24,24	1.34	1 (4%)	35,35,35	1.88	6 (17%)
5	SO4	B	1501	-	4,4,4	0.44	0	6,6,6	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	767(A)	1	12,14,15	0.47	0	15,19,21	0.74	0
3	NAG	B	771(A)	1	12,14,15	0.48	0	15,19,21	0.71	0
3	NAG	B	772(A)	1	12,14,15	0.47	0	15,19,21	0.60	0
3	NAG	B	773(A)	1	12,14,15	0.38	0	15,19,21	0.88	1 (6%)
2	0QG	B	802	1	24,24,24	1.47	2 (8%)	35,35,35	1.88	7 (20%)
5	SO4	C	1502	-	4,4,4	0.43	0	6,6,6	0.61	0
3	NAG	C	767(A)	1	12,14,15	0.46	0	15,19,21	0.94	1 (6%)
3	NAG	C	768(A)	1	12,14,15	0.41	0	15,19,21	0.81	0
3	NAG	C	769(A)	1	12,14,15	0.47	0	15,19,21	0.80	0
3	NAG	C	770(A)	1	12,14,15	0.58	0	15,19,21	0.78	0
3	NAG	C	771(A)	1	12,14,15	0.54	0	15,19,21	0.93	0
2	0QG	C	802	1	24,24,24	1.37	2 (8%)	35,35,35	1.85	5 (14%)
5	SO4	D	1503	-	4,4,4	0.65	0	6,6,6	0.65	0
3	NAG	D	767(A)	1	12,14,15	0.54	0	15,19,21	0.65	0
3	NAG	D	773(A)	1	12,14,15	0.55	0	15,19,21	0.82	0
2	0QG	D	802	1	24,24,24	1.38	1 (4%)	35,35,35	3.07	6 (17%)

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
3	NAG	A	767(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	A	768(A)	1	-	2/6/23/26	0/1/1/1
3	NAG	A	771(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	A	772(A)	1	-	0/6/23/26	0/1/1/1
2	0QG	A	802	1	-	0/32/42/42	0/1/1/1
5	SO4	B	1501	-	-	0/0/0/0	0/0/0/0
3	NAG	B	767(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	B	772(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	B	773(A)	1	-	0/6/23/26	0/1/1/1
2	0QG	B	802	1	-	0/32/42/42	0/1/1/1
5	SO4	C	1502	-	-	0/0/0/0	0/0/0/0
3	NAG	C	767(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	C	768(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	C	769(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	C	770(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	C	771(A)	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0QG	C	802	1	-	0/32/42/42	0/1/1/1
5	SO4	D	1503	-	-	0/0/0/0	0/0/0/0
3	NAG	D	767(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	D	773(A)	1	-	0/6/23/26	0/1/1/1
2	0QG	D	802	1	-	0/32/42/42	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	0QG	C1-N2	6.19	1.48	1.34
2	D	802	0QG	C1-N2	5.65	1.47	1.34
2	A	802	0QG	C1-N2	5.60	1.47	1.34
2	C	802	0QG	C1-N2	5.50	1.47	1.34
2	C	802	0QG	CA1-C1	2.58	1.58	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	0QG	CG1-CB-CA	11.82	131.35	110.00
2	D	802	0QG	CG2-CB-CA	-7.44	96.55	110.00
2	D	802	0QG	O1-C1-N2	-7.00	109.45	122.93
2	C	802	0QG	O1-C1-N2	-6.88	109.69	122.93
2	A	802	0QG	O1-C1-N2	-6.84	109.76	122.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	768(A)	NAG	C8-C7-N2-C2
3	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.