wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:51 AM GMT

PDB ID	:	2BUA
Title	:	CRYSTAL STRUCTURE OF PORCINE DIPEPTIDYL PEPTIDASE IV (CD26) IN COMPLEX WITH A LOW MOLECULAR WEIGHT INHIBITOR.
Authors	:	Nordhoff, S.; Cerezo-Galvez, S.; Feurer, A.; Hill, O.; Matassa, V.G.; Metz, G.; Rummey, C.; Thiemann, M.; Edwards, P.J.
Deposited on	:	2005-06-09
Resolution	:	2.56 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

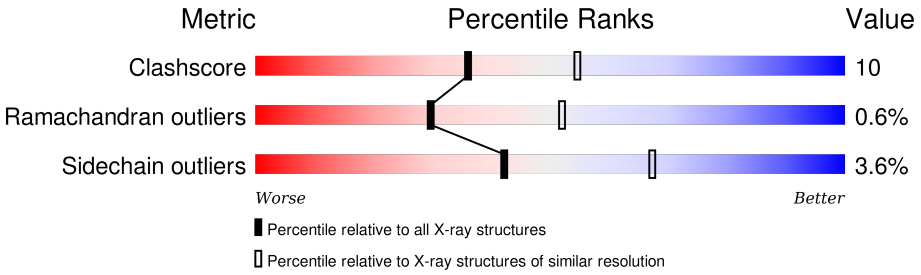
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (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. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	79% 20%
1	B	728	79% 19%
1	C	728	79% 20%
1	D	728	80% 18%

2 Entry composition

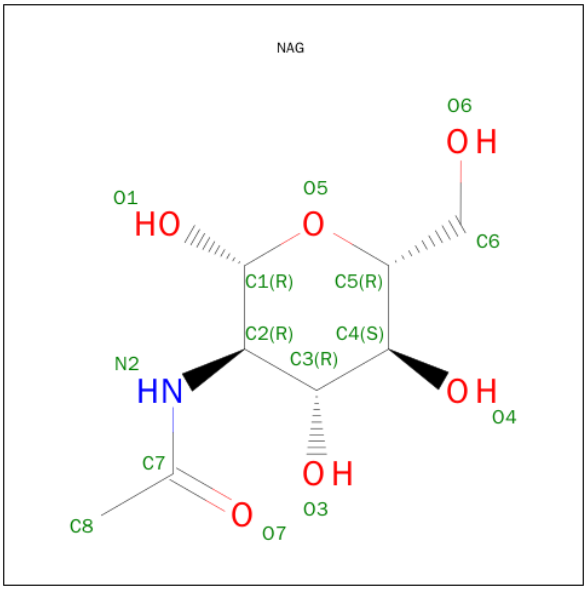
There are 10 unique types of molecules in this entry. The entry contains 25244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIPEPTIDYL PEPTIDASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	0	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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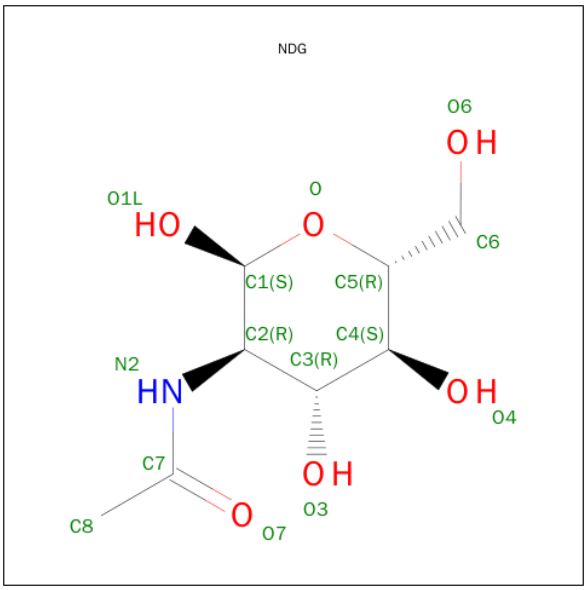
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

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

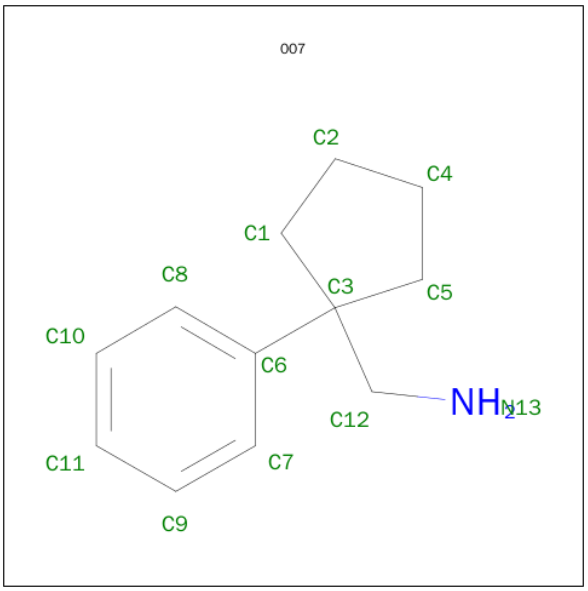
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

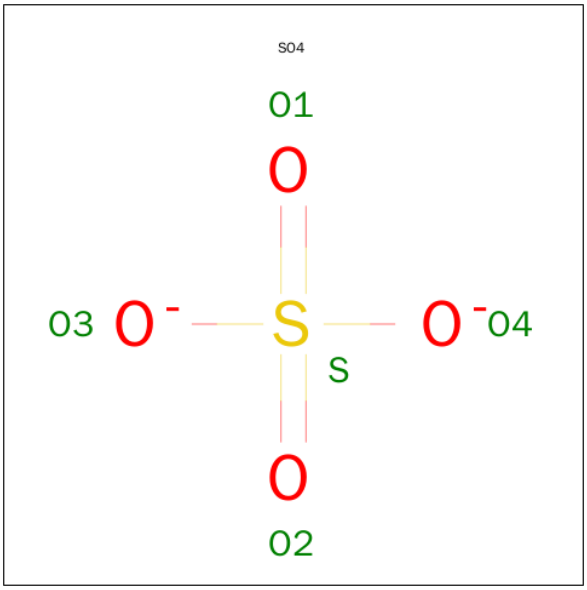
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total C N O 28 16 2 10	0	0
5	D	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is 1-METHYLAMINE-1-BENZYL-CYCLOPENTANE (three-letter code: 007) (formula: $C_{12}H_{17}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 13 12 1	0	0
6	B	1	Total C N 13 12 1	0	0
6	C	1	Total C N 13 12 1	0	0
6	D	1	Total C N 13 12 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	186	Total	O	0	0
			186	186		
10	B	254	Total	O	0	0
			254	254		
10	C	207	Total	O	0	0
			207	207		
10	D	179	Total	O	0	0
			179	179		

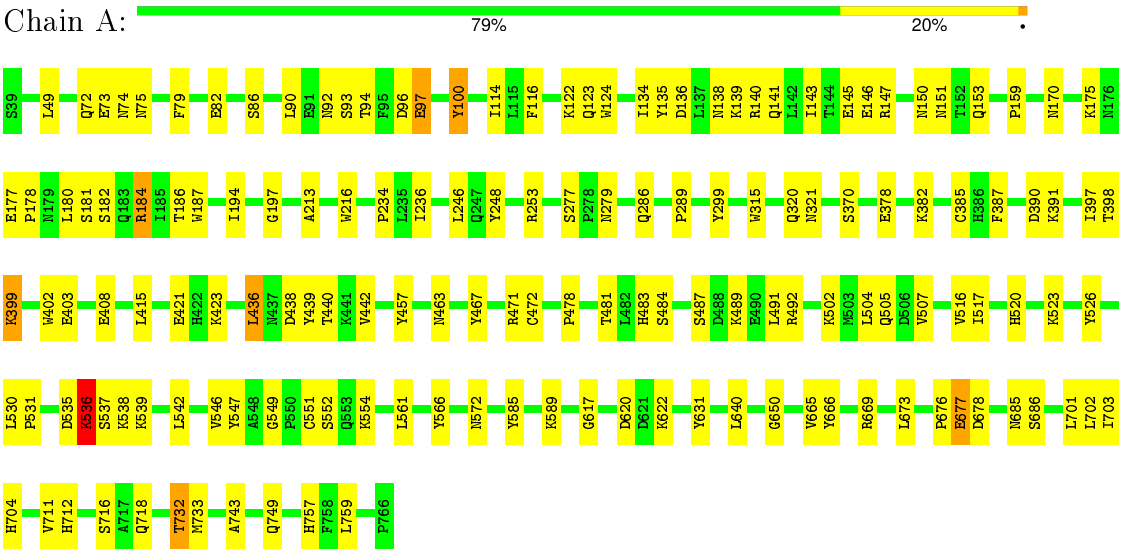
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 was not executed.

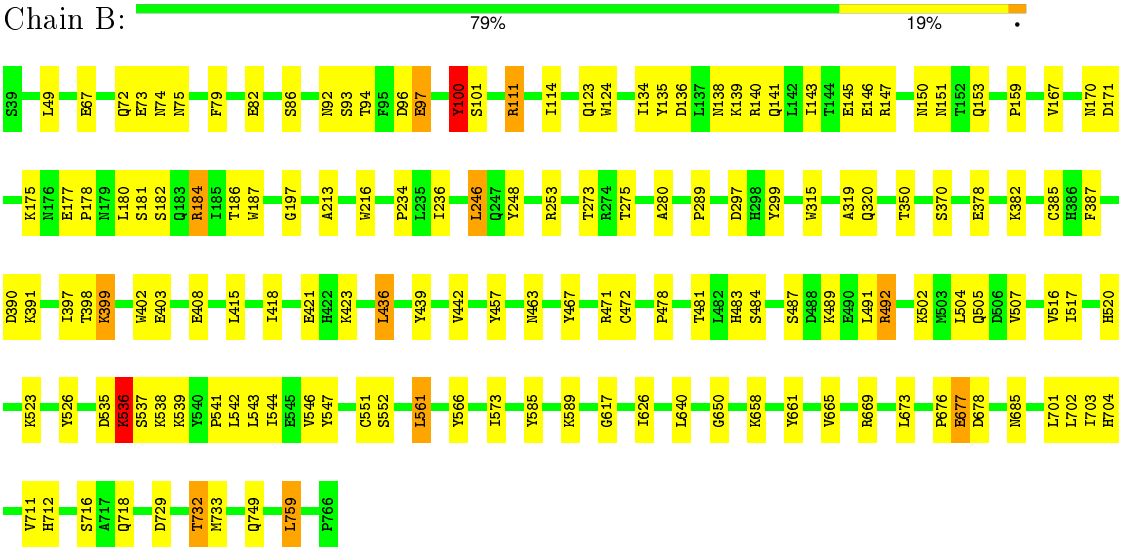
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain A:



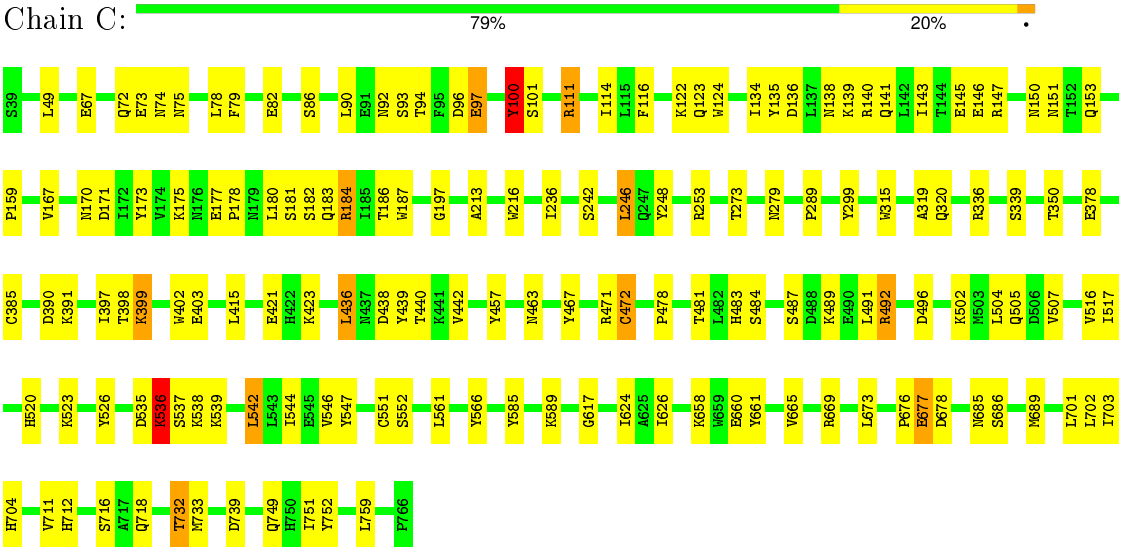
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain B:



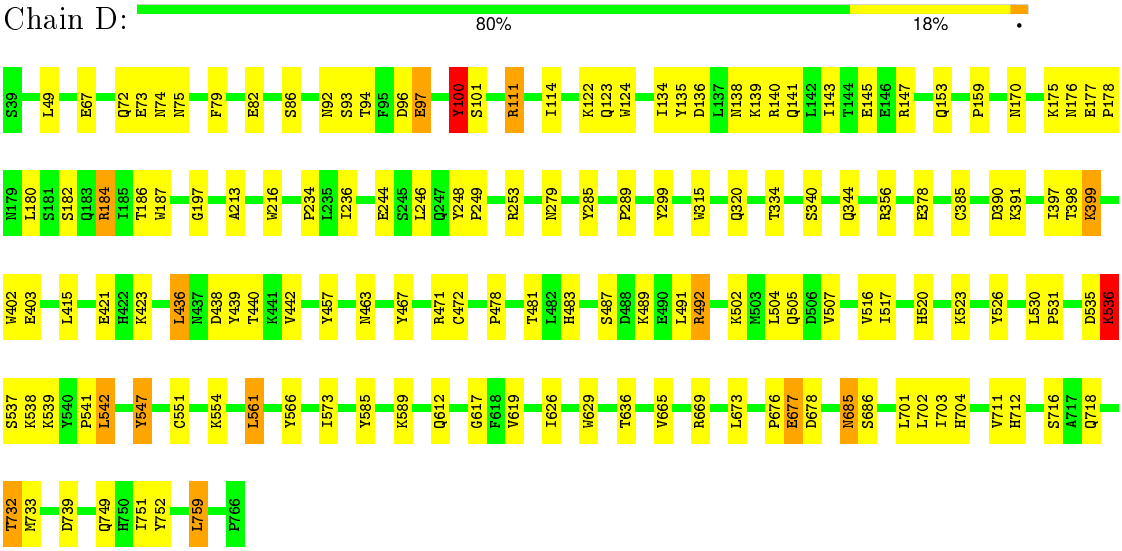
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain C:



• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.42Å 118.13Å 133.32Å 112.40° 94.98° 90.99°	Depositor
Resolution (Å)	20.00 – 2.56	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.56)	Depositor
R_{merge}	0.00	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.220 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25244	wwPDB-VP
Average B, all atoms (Å^2)	47.0	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: 007, NAG, NDG, 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	0.40	0/6141	0.66	3/8353 (0.0%)
1	B	0.39	0/6141	0.66	3/8353 (0.0%)
1	C	0.40	0/6141	0.67	3/8353 (0.0%)
1	D	0.40	0/6141	0.66	3/8353 (0.0%)
All	All	0.40	0/24564	0.66	12/33412 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	492	ARG	NE-CZ-NH1	-15.36	112.62	120.30
1	C	492	ARG	NE-CZ-NH2	14.91	127.76	120.30
1	B	492	ARG	NE-CZ-NH2	-14.49	113.06	120.30
1	A	492	ARG	NE-CZ-NH1	-14.47	113.07	120.30
1	B	492	ARG	NE-CZ-NH1	14.34	127.47	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	5966	0	5663	117	0
1	B	5966	0	5663	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5966	0	5663	121	0
1	D	5966	0	5660	112	0
2	A	42	0	39	2	0
2	B	56	0	52	1	0
2	C	56	0	52	1	0
2	D	14	0	13	1	0
3	A	14	0	13	0	0
3	C	14	0	13	1	0
3	D	14	0	13	0	0
4	A	28	0	25	3	0
4	B	28	0	25	0	0
4	D	28	0	25	3	0
5	A	28	0	25	1	0
5	D	28	0	25	2	0
6	A	13	0	17	1	0
6	B	13	0	17	0	0
6	C	13	0	17	0	0
6	D	13	0	17	0	0
7	A	10	0	0	0	0
7	B	10	0	0	0	0
7	C	10	0	0	0	0
7	D	10	0	0	0	0
8	B	28	0	25	2	0
8	D	56	0	50	3	0
9	C	28	0	25	1	0
10	A	186	0	0	6	0
10	B	254	0	0	8	0
10	C	207	0	0	10	0
10	D	179	0	0	6	0
All	All	25244	0	23137	458	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 10.

The worst 5 of 458 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:253:ARG:HH21	1:D:253:ARG:HH21	1.07	1.00
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.24	0.86
1:A:536:LYS:H	1:A:536:LYS:HD2	1.42	0.84
1:D:536:LYS:HD2	1:D:536:LYS:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LYS:HD2	1:B:536:LYS:H	1.46	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	677 (93%)	45 (6%)	4 (1%)	30	52
1	B	726/728 (100%)	678 (93%)	44 (6%)	4 (1%)	30	52
1	C	726/728 (100%)	676 (93%)	46 (6%)	4 (1%)	30	52
1	D	726/728 (100%)	676 (93%)	46 (6%)	4 (1%)	30	52
All	All	2904/2912 (100%)	2707 (93%)	181 (6%)	16 (1%)	30	52

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	TYR
1	A	536	LYS
1	A	617	GLY
1	B	100	TYR
1	B	536	LYS

5.3.2 Protein sidechains (i)

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%)	631 (97%)	21 (3%)	46	71
1	B	652/652 (100%)	628 (96%)	24 (4%)	41	66
1	C	652/652 (100%)	629 (96%)	23 (4%)	43	68
1	D	652/652 (100%)	627 (96%)	25 (4%)	40	65
All	All	2608/2608 (100%)	2515 (96%)	93 (4%)	42	67

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	702	LEU
1	C	399	LYS
1	D	566	TYR
1	B	732	THR
1	C	111	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	679	ASN
1	C	170	ASN
1	D	520	HIS
1	B	694	ASN
1	B	757	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

18 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	1229	1,4	14,14,15	0.52	0	15,19,21	0.67	0
4	NAG	A	1230	4	14,14,15	0.67	0	15,19,21	0.74	1 (6%)
5	NDG	A	1685	1,5	14,14,15	0.86	0	15,19,21	1.58	3 (20%)
5	NDG	A	1686	5	14,14,15	0.82	1 (7%)	15,19,21	0.95	1 (6%)
8	NDG	B	1092	1,8	14,14,15	0.76	0	15,19,21	1.08	2 (13%)
8	NAG	B	1093	8	14,14,15	0.59	0	15,19,21	1.21	2 (13%)
4	NAG	B	1685	1,4	14,14,15	0.57	0	15,19,21	0.69	0
4	NAG	B	1686	4	14,14,15	0.56	0	15,19,21	0.83	1 (6%)
9	NAG	C	1685	1,9	14,14,15	0.71	0	15,19,21	0.59	0
9	NDG	C	1686	9	14,14,15	0.85	1 (7%)	15,19,21	0.82	0
8	NDG	D	1092	1,8	14,14,15	0.87	1 (7%)	15,19,21	0.89	0
8	NAG	D	1093	8	14,14,15	0.56	0	15,19,21	0.76	0
8	NDG	D	1229	1,8	14,14,15	0.68	0	15,19,21	1.47	3 (20%)
8	NAG	D	1230	8	14,14,15	0.78	1 (7%)	15,19,21	0.74	1 (6%)
5	NDG	D	1321	1,5	14,14,15	1.00	1 (7%)	15,19,21	1.27	3 (20%)
5	NDG	D	1322	5	14,14,15	0.83	1 (7%)	15,19,21	0.96	1 (6%)
4	NAG	D	1685	1,4	14,14,15	0.59	0	15,19,21	0.75	0
4	NAG	D	1686	4	14,14,15	0.57	0	15,19,21	0.95	1 (6%)

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	1229	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1230	4	-	0/6/23/26	0/1/1/1
5	NDG	A	1685	1,5	-	0/6/23/26	0/1/1/1
5	NDG	A	1686	5	-	0/6/23/26	0/1/1/1
8	NDG	B	1092	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1093	8	-	0/6/23/26	0/1/1/1
4	NAG	B	1685	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1686	4	-	0/6/23/26	0/1/1/1
9	NAG	C	1685	1,9	-	0/6/23/26	0/1/1/1
9	NDG	C	1686	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NDG	D	1092	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	1093	8	-	1/6/23/26	0/1/1/1
8	NDG	D	1229	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	1230	8	-	0/6/23/26	0/1/1/1
5	NDG	D	1321	1,5	-	0/6/23/26	0/1/1/1
5	NDG	D	1322	5	-	0/6/23/26	0/1/1/1
4	NAG	D	1685	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	1686	4	-	0/6/23/26	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)
8	D	1230	NAG	C1-C2	2.15	1.55	1.52
5	D	1322	NDG	C1-C2	2.22	1.55	1.52
9	C	1686	NDG	C1-C2	2.22	1.55	1.52
5	A	1686	NDG	C1-C2	2.25	1.55	1.52
8	D	1092	NDG	C1-C2	2.61	1.56	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1685	NDG	C4-C3-C2	-4.07	104.90	111.23
5	A	1685	NDG	C2-N2-C7	-2.93	119.28	123.04
8	B	1093	NAG	C2-N2-C7	-2.92	119.29	123.04
8	B	1093	NAG	C4-C3-C2	-2.85	106.79	111.23
5	D	1321	NDG	C3-C4-C5	-2.74	105.42	110.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	1093	NAG	O7-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1229	NAG	3	0
4	A	1230	NAG	1	0
5	A	1685	NDG	1	0
8	B	1092	NDG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1093	NAG	2	0
9	C	1685	NAG	1	0
8	D	1092	NDG	2	0
8	D	1093	NAG	3	0
5	D	1321	NDG	2	0
5	D	1322	NDG	2	0
4	D	1685	NAG	2	0
4	D	1686	NAG	1	0

5.6 Ligand geometry (i)

27 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	NAG	A	1085	1	14,14,15	0.69	0	15,19,21	0.59	0
3	NDG	A	1092	1	14,14,15	0.75	1 (7%)	15,19,21	0.81	1 (6%)
2	NAG	A	1279	1	14,14,15	0.68	0	15,19,21	0.66	0
2	NAG	A	1321	1	14,14,15	0.57	0	15,19,21	1.17	2 (13%)
6	007	A	1767	-	13,14,14	1.82	3 (23%)	15,19,19	1.08	2 (13%)
7	SO4	A	1768	-	4,4,4	0.26	0	6,6,6	0.08	0
7	SO4	A	1769	-	4,4,4	0.50	0	6,6,6	0.27	0
2	NAG	B	1085	1	14,14,15	0.51	0	15,19,21	0.78	0
2	NAG	B	1229	1	14,14,15	0.53	0	15,19,21	0.78	0
2	NAG	B	1279	1	14,14,15	0.55	0	15,19,21	0.76	1 (6%)
2	NAG	B	1321	1	14,14,15	0.46	0	15,19,21	0.76	1 (6%)
6	007	B	1767	-	13,14,14	1.44	3 (23%)	15,19,19	0.78	0
7	SO4	B	1768	-	4,4,4	0.33	0	6,6,6	0.20	0
7	SO4	B	1769	-	4,4,4	0.44	0	6,6,6	0.12	0
2	NAG	C	1085	1	14,14,15	0.59	0	15,19,21	0.66	0
3	NDG	C	1092	1	14,14,15	0.97	1 (7%)	15,19,21	0.78	0
2	NAG	C	1229	1	14,14,15	0.51	0	15,19,21	0.85	0
2	NAG	C	1279	1	14,14,15	0.63	0	15,19,21	0.80	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	1321	1	14,14,15	0.59	0	15,19,21	0.93	1 (6%)
6	007	C	1767	-	13,14,14	1.70	3 (23%)	15,19,19	0.80	1 (6%)
7	SO4	C	1768	-	4,4,4	0.31	0	6,6,6	0.16	0
7	SO4	C	1769	-	4,4,4	0.46	0	6,6,6	0.13	0
3	NDG	D	1085	1	14,14,15	0.74	0	15,19,21	0.89	0
2	NAG	D	1279	1	14,14,15	0.68	0	15,19,21	0.67	0
6	007	D	1767	-	13,14,14	1.69	3 (23%)	15,19,19	0.99	1 (6%)
7	SO4	D	1768	-	4,4,4	0.31	0	6,6,6	0.13	0
7	SO4	D	1769	-	4,4,4	0.48	0	6,6,6	0.09	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	NAG	A	1085	1	-	0/6/23/26	0/1/1/1
3	NDG	A	1092	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1279	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1321	1	-	0/6/23/26	0/1/1/1
6	007	A	1767	-	-	0/6/18/18	0/2/2/2
7	SO4	A	1768	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1769	-	-	0/0/0/0	0/0/0/0
2	NAG	B	1085	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1229	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1279	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1321	1	-	0/6/23/26	0/1/1/1
6	007	B	1767	-	-	0/6/18/18	0/2/2/2
7	SO4	B	1768	-	-	0/0/0/0	0/0/0/0
7	SO4	B	1769	-	-	0/0/0/0	0/0/0/0
2	NAG	C	1085	1	-	0/6/23/26	0/1/1/1
3	NDG	C	1092	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1229	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1279	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1321	1	-	0/6/23/26	0/1/1/1
6	007	C	1767	-	-	0/6/18/18	0/2/2/2
7	SO4	C	1768	-	-	0/0/0/0	0/0/0/0
7	SO4	C	1769	-	-	0/0/0/0	0/0/0/0
3	NDG	D	1085	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1279	1	-	0/6/23/26	0/1/1/1
6	007	D	1767	-	-	0/6/18/18	0/2/2/2
7	SO4	D	1768	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SO4	D	1769	-	-	0/0/0/0	0/0/0/0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1767	007	C7-C6	2.12	1.42	1.39
3	A	1092	NDG	C1-C2	2.22	1.55	1.52
6	C	1767	007	C7-C6	2.35	1.42	1.39
6	B	1767	007	C8-C6	2.37	1.43	1.39
6	C	1767	007	C8-C6	2.67	1.43	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1321	NAG	C2-N2-C7	-3.19	118.94	123.04
2	A	1321	NAG	C4-C3-C2	-2.41	107.49	111.23
2	B	1321	NAG	C2-N2-C7	-2.34	120.04	123.04
2	B	1279	NAG	C2-N2-C7	-2.21	120.20	123.04
2	C	1279	NAG	C2-N2-C7	-2.02	120.44	123.04

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1092	NDG	O7-C7-N2-C2
3	C	1092	NDG	C8-C7-N2-C2
2	A	1279	NAG	O7-C7-N2-C2
3	C	1092	NDG	O7-C7-N2-C2
2	B	1085	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1279	NAG	1	0
2	A	1321	NAG	1	0
6	A	1767	007	1	0
2	B	1321	NAG	1	0
3	C	1092	NDG	1	0
2	C	1321	NAG	1	0
2	D	1279	NAG	1	0

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 was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.