



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:43 am GMT

PDB ID : 3G0B
Title : Crystal structure of dipeptidyl peptidase IV in complex with TAK-322
Authors : Zhang, Z.; Wallace, M.B.; Feng, J.; Stafford, J.A.; Kaldor, S.W.; Shi, L.; Skene, R.J.; Aertgeerts, K.; Lee, B.; Jennings, A.; Xu, R.; Kassel, D.; Webb, D.R.; Gwaltney, S.L.
Deposited on : 2009-01-27
Resolution : 2.25 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

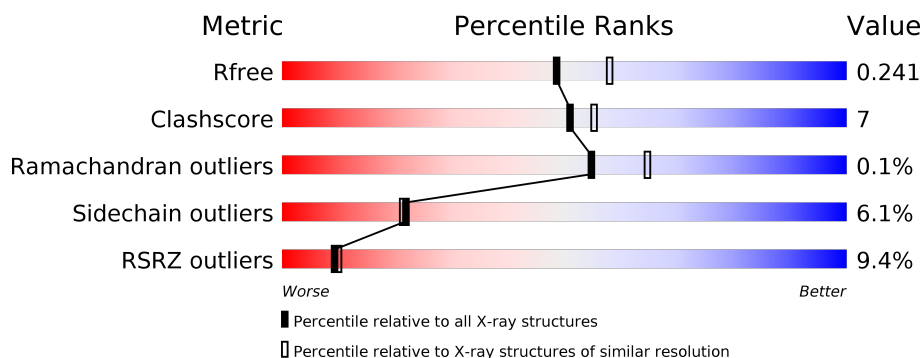
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
R_{free}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	740	<div> <div>10%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>
1	B	740	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
1	C	740	<div> <div>14%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>
1	D	740	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>••</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	804	-	-	-	X
2	NAG	A	811	-	-	-	X
2	NAG	B	808	-	-	-	X
2	NAG	C	807	-	-	-	X
2	NAG	D	807	X	-	-	X
3	NAG	A	802	-	-	-	X
3	NAG	A	805	-	-	-	X
3	NAG	A	809	-	-	-	X
3	NAG	B	803	-	-	-	X
3	NAG	B	804	-	-	-	X
3	NAG	B	805	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24992 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	726	Total	C	N	O	S	0	0	0
			5946	3818	977	1125	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

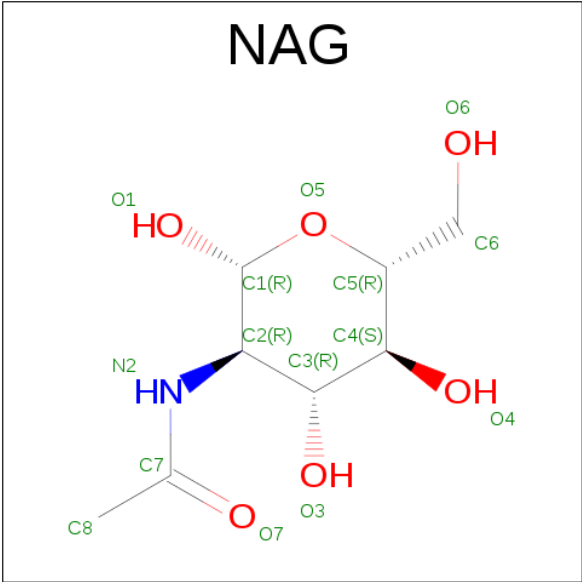
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
A	34	HIS	-	EXPRESSION TAG	UNP P27487
A	35	HIS	-	EXPRESSION TAG	UNP P27487
A	36	HIS	-	EXPRESSION TAG	UNP P27487
A	37	HIS	-	EXPRESSION TAG	UNP P27487
A	38	HIS	-	EXPRESSION TAG	UNP P27487
B	27	ALA	-	EXPRESSION TAG	UNP P27487
B	28	ASP	-	EXPRESSION TAG	UNP P27487
B	29	PRO	-	EXPRESSION TAG	UNP P27487
B	30	GLY	-	EXPRESSION TAG	UNP P27487
B	31	GLY	-	EXPRESSION TAG	UNP P27487
B	32	SER	-	EXPRESSION TAG	UNP P27487
B	33	HIS	-	EXPRESSION TAG	UNP P27487
B	34	HIS	-	EXPRESSION TAG	UNP P27487
B	35	HIS	-	EXPRESSION TAG	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
C	31	GLY	-	EXPRESSION TAG	UNP P27487
C	32	SER	-	EXPRESSION TAG	UNP P27487
C	33	HIS	-	EXPRESSION TAG	UNP P27487
C	34	HIS	-	EXPRESSION TAG	UNP P27487
C	35	HIS	-	EXPRESSION TAG	UNP P27487
C	36	HIS	-	EXPRESSION TAG	UNP P27487
C	37	HIS	-	EXPRESSION TAG	UNP P27487
C	38	HIS	-	EXPRESSION TAG	UNP P27487
D	27	ALA	-	EXPRESSION TAG	UNP P27487
D	28	ASP	-	EXPRESSION TAG	UNP P27487
D	29	PRO	-	EXPRESSION TAG	UNP P27487
D	30	GLY	-	EXPRESSION TAG	UNP P27487
D	31	GLY	-	EXPRESSION TAG	UNP P27487
D	32	SER	-	EXPRESSION TAG	UNP P27487
D	33	HIS	-	EXPRESSION TAG	UNP P27487
D	34	HIS	-	EXPRESSION TAG	UNP P27487
D	35	HIS	-	EXPRESSION TAG	UNP P27487
D	36	HIS	-	EXPRESSION TAG	UNP P27487
D	37	HIS	-	EXPRESSION TAG	UNP P27487
D	38	HIS	-	EXPRESSION TAG	UNP P27487

- 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		
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		
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		

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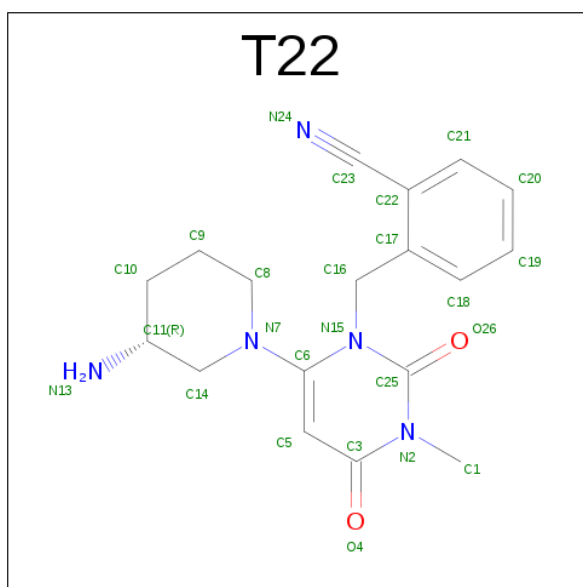
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	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	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		

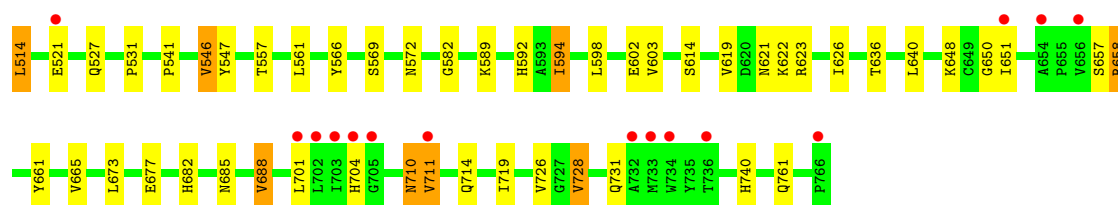
- Molecule 4 is 2-({6-[(3R)-3-AMINOPIPERIDIN-1-YL]-3-METHYL-2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL}METHYL)BENZONITRILE (three-letter code: T22) (formula: C₁₈H₂₁N₅O₂).



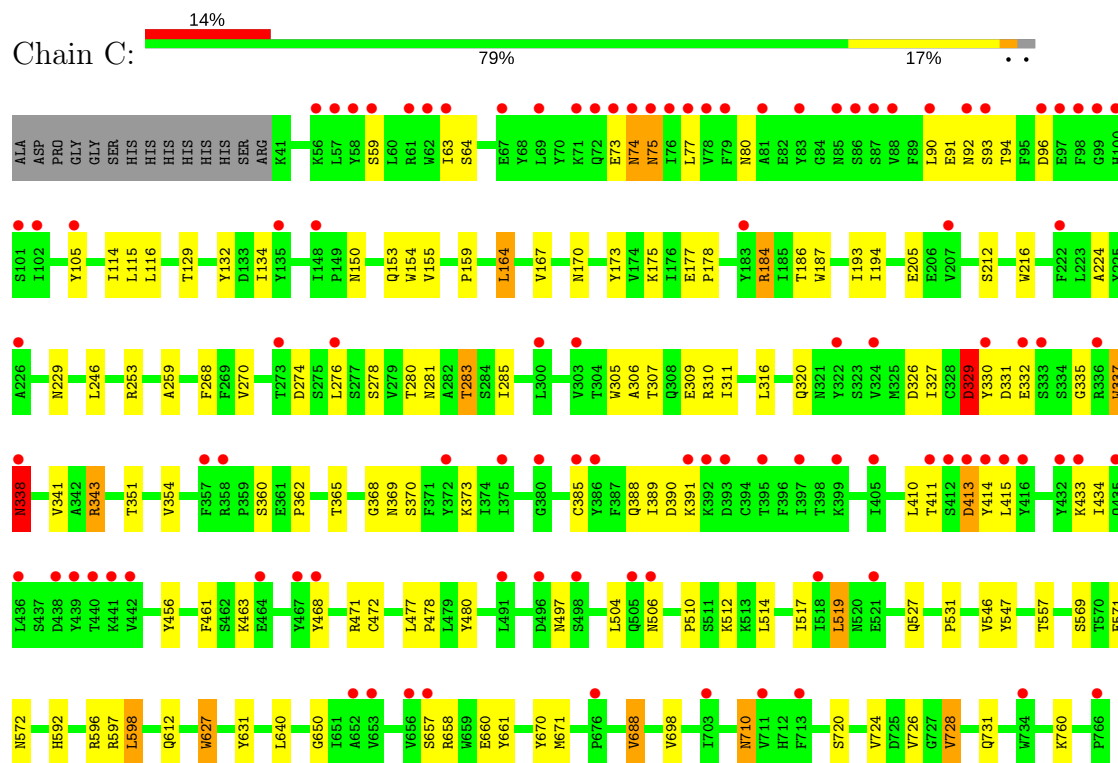
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	18	5	2		
4	B	1	Total	C	N	O	0	0
			25	18	5	2		
4	C	1	Total	C	N	O	0	0
			25	18	5	2		
4	D	1	Total	C	N	O	0	0
			25	18	5	2		

- Molecule 5 is water.

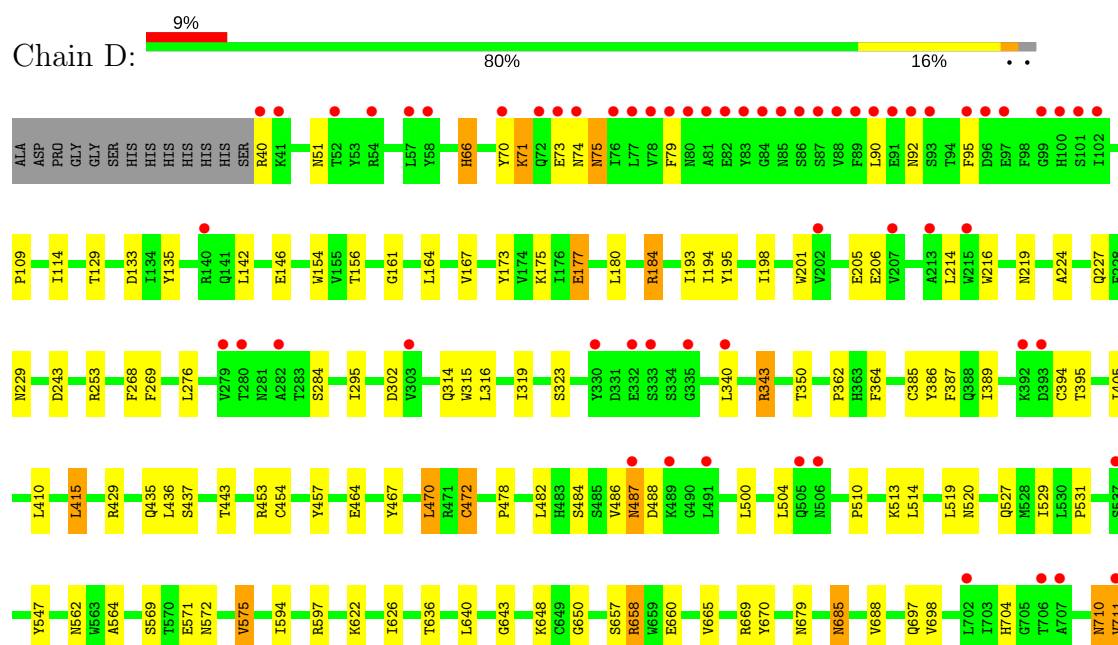
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total	O	0	0
			29	29		
5	B	509	Total	O	0	0
			509	509		
5	C	4	Total	O	0	0
			4	4		
5	D	15	Total	O	0	0
			15	15		

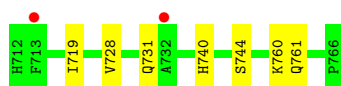


• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.69Å 122.40Å 144.01Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	35.00 – 2.25 34.62 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (35.00-2.25) 97.0 (34.62-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.242 0.204 , 0.241	Depositor DCC
R_{free} test set	8844 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24992	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: T22, 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	0.49	0/6129	0.63	0/8336
1	B	0.48	0/6190	0.63	2/8419 (0.0%)
1	C	0.82	23/6118 (0.4%)	0.67	9/8322 (0.1%)
1	D	0.48	0/6129	0.62	1/8336 (0.0%)
All	All	0.59	23/24566 (0.1%)	0.64	12/33413 (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	C	0	1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	338	ASN	CG-ND2	22.47	1.89	1.32
1	C	329	ASP	CG-OD1	17.61	1.65	1.25
1	C	343	ARG	CZ-NH2	17.20	1.55	1.33
1	C	177	GLU	CD-OE2	13.47	1.40	1.25
1	C	177	GLU	CD-OE1	11.77	1.38	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	329	ASP	CB-CG-OD1	-19.59	100.67	118.30
1	C	343	ARG	NE-CZ-NH1	-10.23	115.19	120.30
1	C	274	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	C	329	ASP	OD1-CG-OD2	6.81	136.24	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	415	LEU	CA-CB-CG	6.75	130.83	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	338	ASN	Sidechain

5.2 Too-close contacts [i](#)

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	5957	0	5679	84	0
1	B	6013	0	5720	73	0
1	C	5946	0	5666	84	0
1	D	5957	0	5676	83	0
2	A	56	0	52	4	0
2	B	56	0	52	5	0
2	C	56	0	52	3	0
2	D	70	0	65	4	0
3	A	112	0	100	6	0
3	B	56	0	50	2	0
3	C	28	0	25	2	0
3	D	28	0	25	5	0
4	A	25	0	21	1	0
4	B	25	0	21	1	0
4	C	25	0	21	1	0
4	D	25	0	21	1	0
5	A	29	0	0	0	0
5	B	509	0	0	1	0
5	C	4	0	0	0	0
5	D	15	0	0	0	0
All	All	24992	0	23246	312	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 7.

The worst 5 of 312 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:A:229:ASN:HD21	3:A:805:NAG:C1	1.12	1.58
1:C:329:ASP:CG	1:C:329:ASP:OD1	1.65	1.31
1:C:338:ASN:ND2	1:C:338:ASN:CG	1.89	1.26
1:A:229:ASN:ND2	3:A:805:NAG:C1	1.95	1.25
1:D:229:ASN:HD21	3:D:804:NAG:C1	1.69	1.04

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	725/740 (98%)	697 (96%)	28 (4%)	0	100	100
1	B	731/740 (99%)	704 (96%)	26 (4%)	1 (0%)	55	65
1	C	724/740 (98%)	690 (95%)	32 (4%)	2 (0%)	44	50
1	D	725/740 (98%)	692 (95%)	33 (5%)	0	100	100
All	All	2905/2960 (98%)	2783 (96%)	119 (4%)	3 (0%)	55	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	714	GLN
1	C	73	GLU
1	C	463	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	652/662 (98%)	613 (94%)	39 (6%)	22	22
1	B	658/662 (99%)	610 (93%)	48 (7%)	16	15
1	C	651/662 (98%)	617 (95%)	34 (5%)	27	29
1	D	652/662 (98%)	613 (94%)	39 (6%)	22	22
All	All	2613/2648 (99%)	2453 (94%)	160 (6%)	22	21

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	547	TYR
1	C	75	ASN
1	D	514	LEU
1	B	589	LYS
1	B	688	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	572	ASN
1	C	119	ASN
1	D	487	ASN
1	B	592	HIS
1	C	74	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

16 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	802	1,3	14,14,15	0.51	0	15,19,21	1.87	2 (13%)
3	NAG	A	803	3	14,14,15	0.57	0	15,19,21	1.25	1 (6%)
3	NAG	A	805	3	14,14,15	0.70	0	15,19,21	1.44	2 (13%)
3	NAG	A	806	3	14,14,15	0.44	0	15,19,21	1.57	3 (20%)
3	NAG	A	807	3	14,14,15	0.59	0	15,19,21	1.66	3 (20%)
3	NAG	A	808	3	14,14,15	0.54	0	15,19,21	0.57	0
3	NAG	A	809	3	14,14,15	0.55	0	15,19,21	1.71	3 (20%)
3	NAG	A	810	3	14,14,15	0.64	0	15,19,21	1.18	1 (6%)
3	NAG	B	803	3	14,14,15	0.51	0	15,19,21	0.95	1 (6%)
3	NAG	B	804	3	14,14,15	0.49	0	15,19,21	0.90	1 (6%)
3	NAG	B	805	3	14,14,15	0.69	0	15,19,21	1.29	2 (13%)
3	NAG	B	806	3	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
3	NAG	C	803	3	14,14,15	0.61	0	15,19,21	1.03	1 (6%)
3	NAG	C	804	3	14,14,15	0.50	0	15,19,21	1.70	3 (20%)
3	NAG	D	804	3	14,14,15	0.65	0	15,19,21	1.83	2 (13%)
3	NAG	D	805	3	14,14,15	0.54	0	15,19,21	1.38	3 (20%)

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	802	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	803	3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	3	-	0/6/23/26	0/1/1/1
3	NAG	A	806	3	-	0/6/23/26	0/1/1/1
3	NAG	A	807	3	-	0/6/23/26	0/1/1/1
3	NAG	A	808	3	-	0/6/23/26	0/1/1/1
3	NAG	A	809	3	-	0/6/23/26	0/1/1/1
3	NAG	A	810	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	803	3	-	0/6/23/26	0/1/1/1
3	NAG	B	804	3	-	0/6/23/26	0/1/1/1
3	NAG	B	805	3	-	0/6/23/26	0/1/1/1
3	NAG	B	806	3	-	0/6/23/26	0/1/1/1
3	NAG	C	803	3	-	0/6/23/26	0/1/1/1
3	NAG	C	804	3	-	0/6/23/26	0/1/1/1
3	NAG	D	804	3	-	0/6/23/26	0/1/1/1
3	NAG	D	805	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	804	NAG	O5-C1-C2	-4.64	105.01	111.47
3	A	807	NAG	O5-C1-C2	-3.91	106.04	111.47
3	A	809	NAG	O5-C1-C2	-3.56	106.52	111.47
3	A	805	NAG	C1-O5-C5	-3.54	107.29	112.17
3	B	805	NAG	O5-C1-C2	-3.33	106.84	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	805	NAG	2	0
3	A	807	NAG	1	0
3	A	809	NAG	3	0
3	A	810	NAG	1	0
3	B	805	NAG	2	0
3	C	803	NAG	2	0
3	D	804	NAG	5	0

5.6 Ligand geometry

21 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
4	T22	A	800	-	22,27,27	1.92	1 (4%)	26,38,38	1.40	4 (15%)
2	NAG	A	801	-	14,14,15	0.51	0	15,19,21	0.69	0
2	NAG	A	804	-	14,14,15	0.61	0	15,19,21	0.87	0
2	NAG	A	811	-	14,14,15	0.53	0	15,19,21	1.46	4 (26%)
2	NAG	A	812	-	14,14,15	0.47	0	15,19,21	0.72	0
4	T22	B	800	-	22,27,27	1.92	1 (4%)	26,38,38	1.40	4 (15%)
2	NAG	B	801	-	14,14,15	0.46	0	15,19,21	1.05	1 (6%)
2	NAG	B	802	-	14,14,15	0.54	0	15,19,21	1.28	2 (13%)
2	NAG	B	807	-	14,14,15	0.48	0	15,19,21	0.88	1 (6%)
2	NAG	B	808	-	14,14,15	0.54	0	15,19,21	1.27	2 (13%)
4	T22	C	800	-	22,27,27	1.92	1 (4%)	26,38,38	1.40	4 (15%)
2	NAG	C	802	-	14,14,15	0.57	0	15,19,21	1.41	2 (13%)
2	NAG	C	805	-	14,14,15	0.51	0	15,19,21	0.88	0
2	NAG	C	806	1	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
2	NAG	C	807	-	14,14,15	0.63	0	15,19,21	1.49	2 (13%)
4	T22	D	800	-	22,27,27	1.91	1 (4%)	26,38,38	1.39	4 (15%)
2	NAG	D	802	1	14,14,15	1.18	1 (7%)	15,19,21	1.79	5 (33%)
2	NAG	D	803	-	14,14,15	0.60	0	15,19,21	1.31	2 (13%)
2	NAG	D	806	1	14,14,15	0.75	0	15,19,21	1.41	2 (13%)
2	NAG	D	807	1	14,14,15	0.54	0	15,19,21	1.24	2 (13%)
2	NAG	D	808	-	14,14,15	0.47	0	15,19,21	1.21	2 (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
4	T22	A	800	-	-	0/10/20/20	0/3/3/3
2	NAG	A	801	-	-	0/6/23/26	0/1/1/1
2	NAG	A	804	-	-	0/6/23/26	0/1/1/1
2	NAG	A	811	-	-	0/6/23/26	0/1/1/1
2	NAG	A	812	-	-	1/6/23/26	0/1/1/1
4	T22	B	800	-	-	0/10/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	801	-	-	0/6/23/26	0/1/1/1
2	NAG	B	802	-	-	0/6/23/26	0/1/1/1
2	NAG	B	807	-	-	0/6/23/26	0/1/1/1
2	NAG	B	808	-	-	0/6/23/26	0/1/1/1
4	T22	C	800	-	-	0/10/20/20	0/3/3/3
2	NAG	C	802	-	-	0/6/23/26	0/1/1/1
2	NAG	C	805	-	-	0/6/23/26	0/1/1/1
2	NAG	C	806	1	-	0/6/23/26	0/1/1/1
2	NAG	C	807	-	-	0/6/23/26	0/1/1/1
4	T22	D	800	-	-	0/10/20/20	0/3/3/3
2	NAG	D	802	1	-	0/6/23/26	0/1/1/1
2	NAG	D	803	-	-	0/6/23/26	0/1/1/1
2	NAG	D	806	1	-	0/6/23/26	0/1/1/1
2	NAG	D	807	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	808	-	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	800	T22	C22-C23	-8.14	1.31	1.44
4	A	800	T22	C22-C23	-8.14	1.31	1.44
4	D	800	T22	C22-C23	-8.13	1.31	1.44
4	C	800	T22	C22-C23	-8.12	1.31	1.44
2	D	802	NAG	O5-C1	-4.01	1.37	1.43

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	NAG	O5-C1-C2	-3.38	106.77	111.47
2	B	808	NAG	O5-C1-C2	-3.27	106.92	111.47
2	B	802	NAG	O5-C1-C2	-2.82	107.55	111.47
2	D	808	NAG	O5-C1-C2	-2.49	108.00	111.47
2	D	802	NAG	O5-C1-C2	-2.47	108.04	111.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	807	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	812	NAG	O7-C7-N2-C2

There are no ring outliers.

16 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	T22	1	0
2	A	801	NAG	1	0
2	A	811	NAG	3	0
4	B	800	T22	1	0
2	B	801	NAG	1	0
2	B	802	NAG	1	0
2	B	807	NAG	1	0
2	B	808	NAG	2	0
4	C	800	T22	1	0
2	C	802	NAG	1	0
2	C	805	NAG	1	0
2	C	807	NAG	1	0
4	D	800	T22	1	0
2	D	803	NAG	1	0
2	D	807	NAG	1	0
2	D	808	NAG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/740 (98%)	0.47	71 (9%) 8 9	41, 50, 64, 77	0
1	B	733/740 (99%)	0.27	38 (5%) 28 32	38, 50, 64, 77	0
1	C	726/740 (98%)	0.79	101 (13%) 3 3	44, 51, 73, 88	0
1	D	727/740 (98%)	0.50	63 (8%) 11 12	43, 50, 66, 79	0
All	All	2913/2960 (98%)	0.51	273 (9%) 9 10	38, 50, 67, 88	0

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	10.6
1	C	86	SER	7.6
1	C	77	LEU	7.5
1	C	97	GLU	6.8
1	D	81	ALA	6.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	809	14/15	0.85	0.29	5.70	99,102,103,105	0
3	NAG	B	803	14/15	0.65	0.31	5.60	116,118,119,119	0
3	NAG	B	804	14/15	0.58	0.41	5.20	117,119,119,119	0
3	NAG	A	805	14/15	0.92	0.23	3.82	61,66,68,69	0
3	NAG	B	805	14/15	0.85	0.20	3.31	69,76,79,82	0
3	NAG	A	802	14/15	0.82	0.34	3.24	73,78,81,85	0
3	NAG	D	804	14/15	0.87	0.20	1.53	74,77,79,81	0
3	NAG	C	803	14/15	0.91	0.12	-1.48	54,58,60,62	0
3	NAG	A	803	14/15	0.75	0.43	-	88,91,91,91	0
3	NAG	C	804	14/15	0.89	0.26	-	64,65,66,67	0
3	NAG	A	806	14/15	0.86	0.29	-	71,71,74,74	0
3	NAG	D	805	14/15	0.75	0.43	-	80,85,87,87	0
3	NAG	A	807	14/15	0.62	0.23	-	97,101,102,102	0
3	NAG	B	806	14/15	0.65	0.39	-	81,85,86,87	0
3	NAG	A	808	14/15	0.78	0.29	-	102,103,103,103	0
3	NAG	A	810	14/15	0.60	0.51	-	106,107,108,108	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	811	14/15	0.79	0.41	8.94	71,75,77,78	0
2	NAG	B	808	14/15	0.69	0.38	7.76	90,92,92,92	0
2	NAG	A	804	14/15	0.53	0.43	6.88	97,98,99,99	0
2	NAG	D	807	14/15	0.82	0.37	6.46	73,75,80,80	0
2	NAG	C	807	14/15	0.57	0.41	2.17	89,91,92,92	0
2	NAG	C	806	14/15	0.83	0.29	1.59	71,75,78,78	0
4	T22	A	800	25/25	0.95	0.23	-0.07	48,50,51,52	0
2	NAG	B	801	14/15	0.70	0.25	-0.13	84,86,86,87	0
4	T22	D	800	25/25	0.93	0.15	-0.59	48,50,51,52	0
2	NAG	A	801	14/15	0.74	0.17	-0.75	94,97,97,98	0
4	T22	B	800	25/25	0.94	0.17	-1.10	48,50,51,52	0
4	T22	C	800	25/25	0.96	0.14	-1.53	48,50,51,52	0
2	NAG	D	803	14/15	0.75	0.33	-	84,85,86,86	0
2	NAG	B	802	14/15	0.78	0.27	-	88,89,90,90	0
2	NAG	A	812	14/15	0.58	0.50	-	111,112,114,114	0
2	NAG	D	802	14/15	0.80	0.32	-	66,69,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	807	14/15	0.70	0.13	-	93,94,95,96	0
2	NAG	C	805	14/15	0.81	0.16	-	92,95,96,96	0
2	NAG	C	802	14/15	0.63	0.21	-	88,90,90,90	0
2	NAG	D	806	14/15	0.77	0.23	-	70,74,75,76	0
2	NAG	D	808	14/15	0.72	0.30	-	91,93,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.