



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:22 am GMT

PDB ID : 2BGN
Title : HIV-1 TAT PROTEIN DERIVED N-TERMINAL NONAPEPTIDE TRP2-TAT (1-9) BOUND TO THE ACTIVE SITE OF DIPEPTIDYL PEPTIDASE IV (CD26)
Authors : Weihofen, W.A.; Liu, J.; Reutter, W.; Saenger, W.; Fan, H.
Deposited on : 2005-01-03
Resolution : 3.15 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

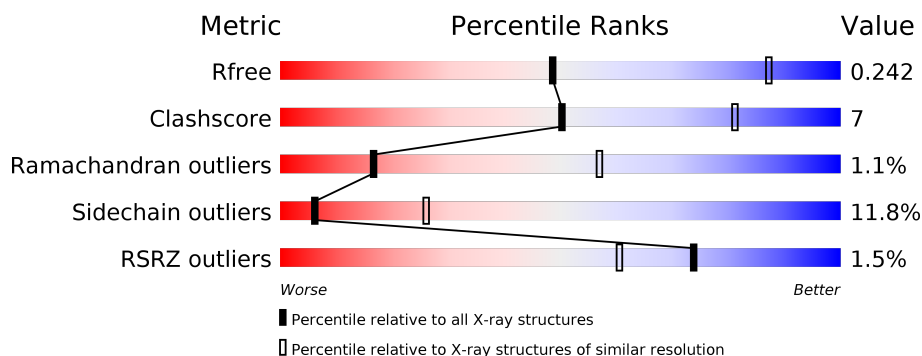
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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	728	<div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	B	728	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	C	728	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	D	728	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
2	E	363	<div> <div>6%</div> <div>63%</div> <div>28%</div> <div>...</div> </div>
2	F	363	<div> <div>3%</div> <div>58%</div> <div>33%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	363	
2	H	363	
3	W	9	
3	X	9	
3	Y	9	
3	Z	9	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	800	-	-	-	X
5	NAG	A	850	-	-	-	X
5	NAG	B	821	-	-	-	X
5	NAG	B	850	-	-	-	X
5	NAG	C	850	-	-	-	X
5	NAG	D	821	-	-	-	X
5	NAG	D	850	-	-	-	X
7	NAG	A	840	X	-	-	-
7	NAG	A	860	-	-	-	X
7	NAG	B	860	X	-	-	X
7	NAG	C	860	-	-	-	X
7	NAG	D	860	X	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 36096 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
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	C	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	D	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			
2	F	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			
2	G	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			
2	H	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	ASP	ASN	CONFLICT SEE REMARK 9	UNP P56658
E	32	LYS	ARG	CONFLICT SEE REMARK 9	UNP P56658
E	33	ARG	LYS	CONFLICT SEE REMARK 9	UNP P56658
E	47	LEU	GLN	CONFLICT	UNP P56658
E	57	THR	SER	CONFLICT SEE REMARK 9	UNP P56658
E	60	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
E	77	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
E	79	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658

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Chain	Residue	Modelled	Actual	Comment	Reference
E	199	GLN	LYS	VARIANT	UNP P56658
E	246	THR	ALA	VARIANT	UNP P56658
E	261	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
E	279	ALA	PRO	CONFLICT SEE REMARK 9	UNP P56658
E	281	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
E	313	LYS	ASN	CONFLICT SEE REMARK 9	UNP P56658
E	314	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
E	352	ARG	GLY	VARIANT	UNP P56658
F	8	ASP	ASN	CONFLICT SEE REMARK 9	UNP P56658
F	32	LYS	ARG	CONFLICT SEE REMARK 9	UNP P56658
F	33	ARG	LYS	CONFLICT SEE REMARK 9	UNP P56658
F	47	LEU	GLN	CONFLICT	UNP P56658
F	57	THR	SER	CONFLICT SEE REMARK 9	UNP P56658
F	60	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
F	77	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
F	79	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
F	199	GLN	LYS	VARIANT	UNP P56658
F	246	THR	ALA	VARIANT	UNP P56658
F	261	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
F	279	ALA	PRO	CONFLICT SEE REMARK 9	UNP P56658
F	281	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
F	313	LYS	ASN	CONFLICT SEE REMARK 9	UNP P56658
F	314	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
F	352	ARG	GLY	VARIANT	UNP P56658
G	8	ASP	ASN	CONFLICT SEE REMARK 9	UNP P56658
G	32	LYS	ARG	CONFLICT SEE REMARK 9	UNP P56658
G	33	ARG	LYS	CONFLICT SEE REMARK 9	UNP P56658
G	47	LEU	GLN	CONFLICT	UNP P56658
G	57	THR	SER	CONFLICT SEE REMARK 9	UNP P56658
G	60	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
G	77	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
G	79	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
G	199	GLN	LYS	VARIANT	UNP P56658
G	246	THR	ALA	VARIANT	UNP P56658
G	261	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
G	279	ALA	PRO	CONFLICT SEE REMARK 9	UNP P56658
G	281	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
G	313	LYS	ASN	CONFLICT SEE REMARK 9	UNP P56658
G	314	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
G	352	ARG	GLY	VARIANT	UNP P56658
H	8	ASP	ASN	CONFLICT SEE REMARK 9	UNP P56658
H	32	LYS	ARG	CONFLICT SEE REMARK 9	UNP P56658

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Chain	Residue	Modelled	Actual	Comment	Reference
H	33	ARG	LYS	CONFLICT SEE REMARK 9	UNP P56658
H	47	LEU	GLN	CONFLICT	UNP P56658
H	57	THR	SER	CONFLICT SEE REMARK 9	UNP P56658
H	60	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
H	77	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
H	79	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
H	199	GLN	LYS	VARIANT	UNP P56658
H	246	THR	ALA	VARIANT	UNP P56658
H	261	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
H	279	ALA	PRO	CONFLICT SEE REMARK 9	UNP P56658
H	281	ILE	VAL	CONFLICT SEE REMARK 9	UNP P56658
H	313	LYS	ASN	CONFLICT SEE REMARK 9	UNP P56658
H	314	ASP	GLU	CONFLICT SEE REMARK 9	UNP P56658
H	352	ARG	GLY	VARIANT	UNP P56658

- Molecule 3 is a protein called TAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	6	Total	C	N	O	S	0	0	0
			51	35	7	8	1			
3	X	6	Total	C	N	O	S	0	0	0
			51	35	7	8	1			
3	Y	6	Total	C	N	O	S	0	0	0
			51	35	7	8	1			
3	Z	6	Total	C	N	O	S	0	0	0
			51	35	7	8	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	2	TRP	ASP	ENGINEERED MUTATION	UNP P12506
X	2	TRP	ASP	ENGINEERED MUTATION	UNP P12506
Y	2	TRP	ASP	ENGINEERED MUTATION	UNP P12506
Z	2	TRP	ASP	ENGINEERED MUTATION	UNP P12506

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		
4	C	3	Total	C	N	O	0	0
			38	22	2	14		

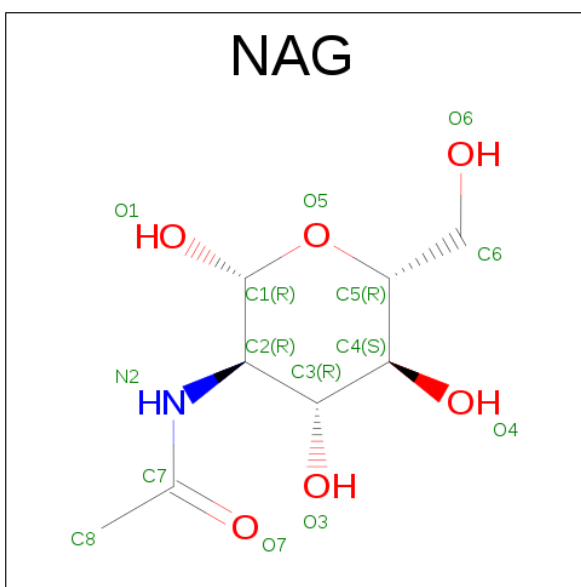
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			50	28	2	20		
6	B	4	Total	C	N	O	0	0
			50	28	2	20		
6	C	4	Total	C	N	O	0	0
			50	28	2	20		
6	D	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- 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
			24	14	1	9		
8	D	2	Total	C	N	O	0	0
			24	14	1	9		

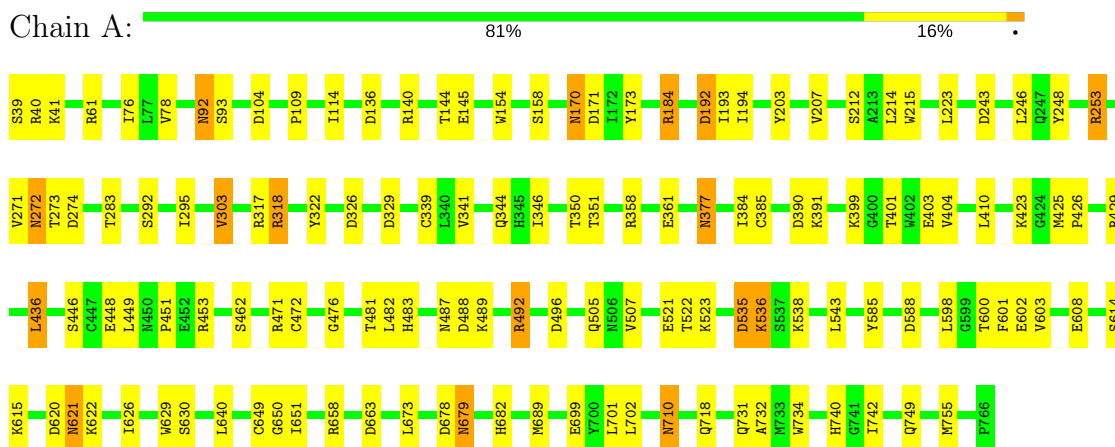
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	Zn	0	0
			1	1		
9	G	1	Total	Zn	0	0
			1	1		
9	F	1	Total	Zn	0	0
			1	1		
9	E	1	Total	Zn	0	0
			1	1		

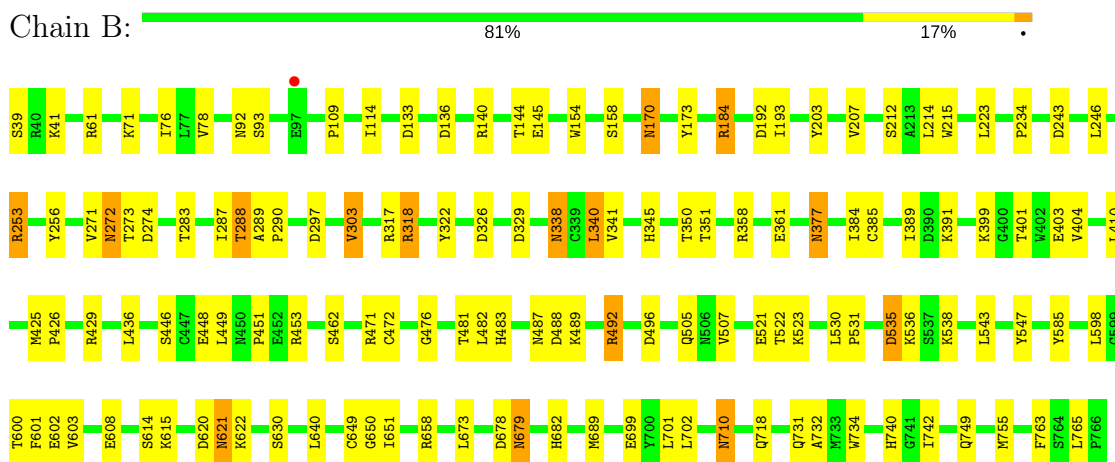
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

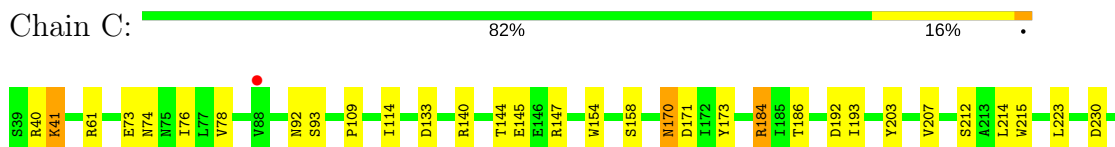
• Molecule 1: DIPEPTIDYL PEPTIDASE IV



• Molecule 1: DIPEPTIDYL PEPTIDASE IV



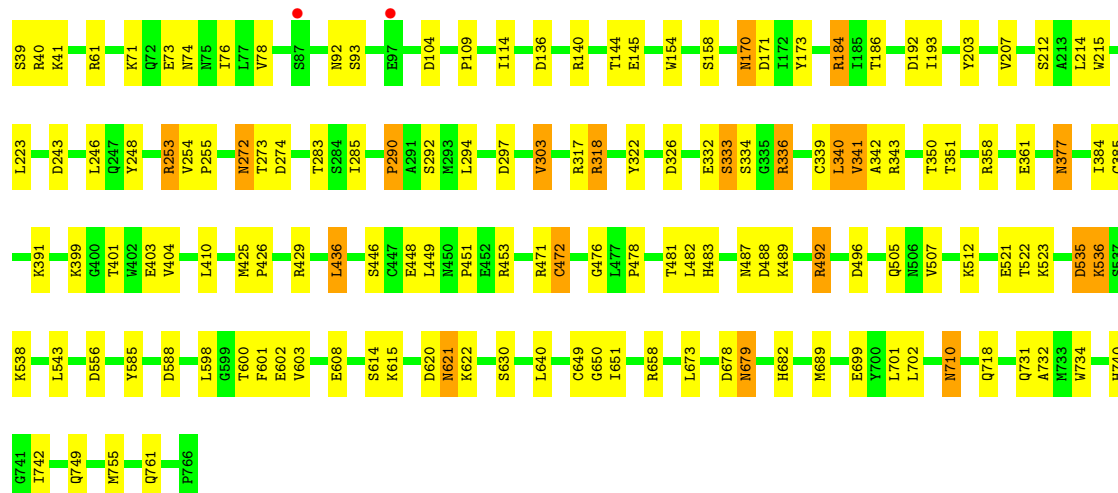
• Molecule 1: DIPEPTIDYL PEPTIDASE IV





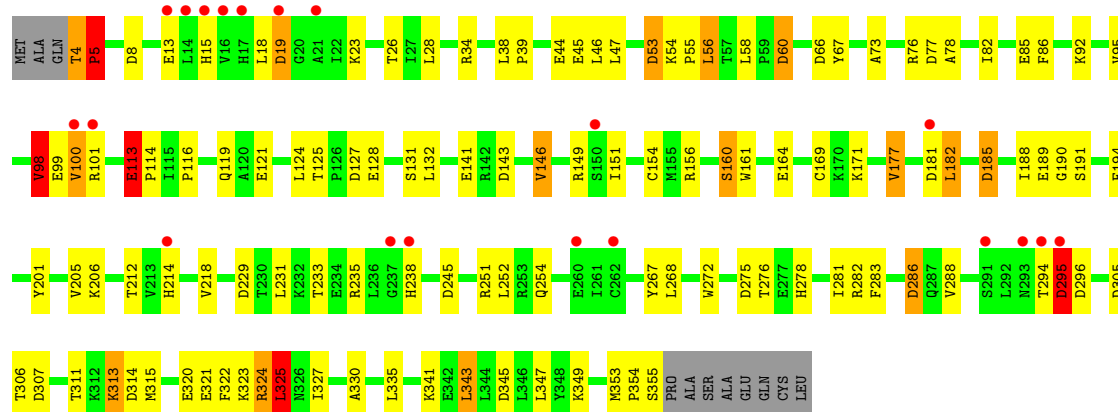
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain D: 80% 17%



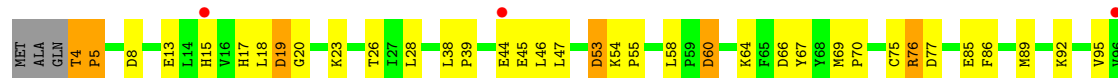
• Molecule 2: ADENOSINE DEAMINASE

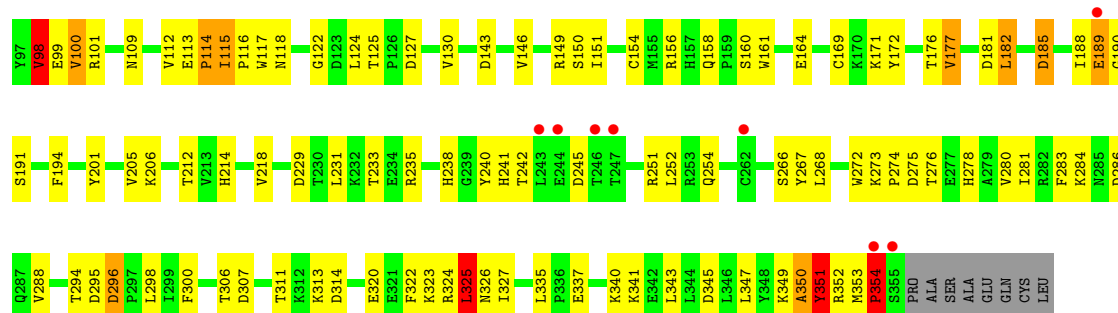
Chain E: 63% 28% 6%



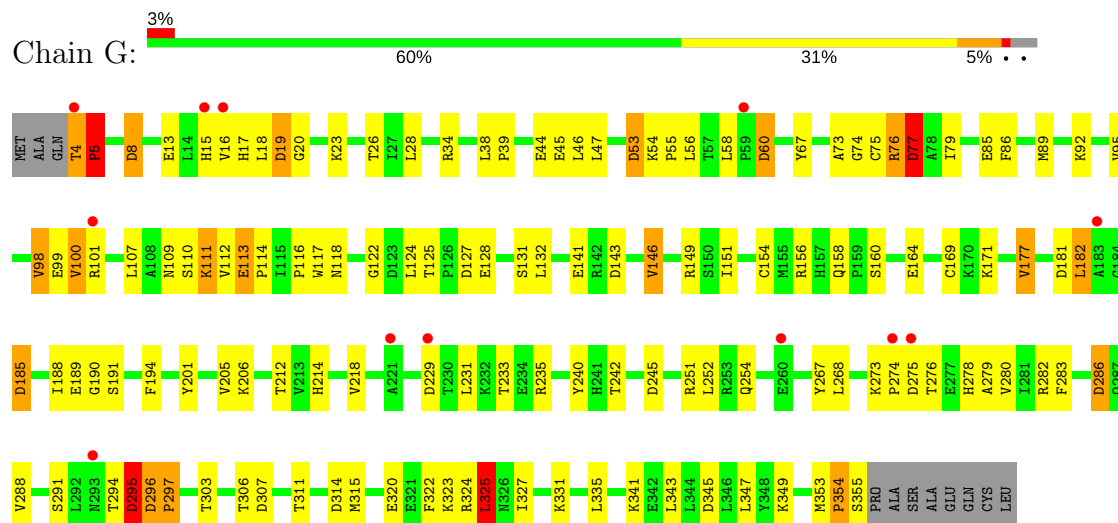
• Molecule 2: ADENOSINE DEAMINASE

Chain F: 58% 33% 3%

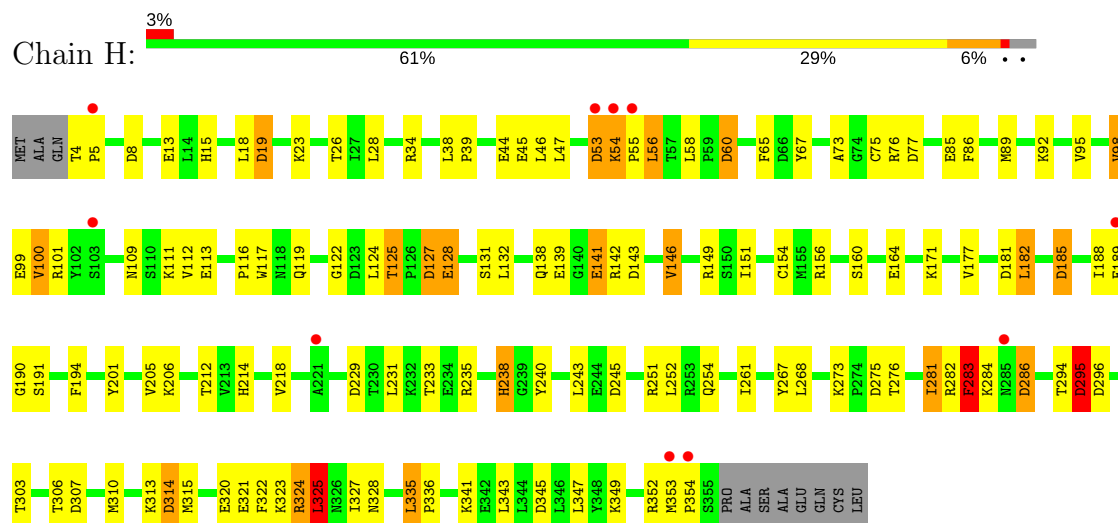




• Molecule 2: ADENOSINE DEAMINASE



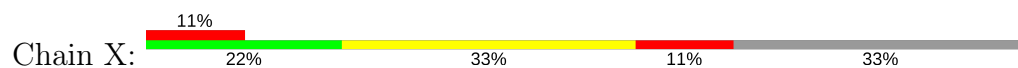
• Molecule 2: ADENOSINE DEAMINASE



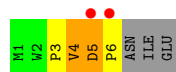
• Molecule 3: TAT PROTEIN



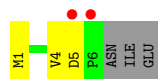
● Molecule 3: TAT PROTEIN



● Molecule 3: TAT PROTEIN



● Molecule 3: TAT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.94Å 170.27Å 239.20Å 90.00° 100.93° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15 29.74 – 3.15	Depositor EDS
% Data completeness (in resolution range)	89.6 (30.00-3.15) 89.6 (29.74-3.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.227 , 0.247 0.221 , 0.242	Depositor DCC
R_{free} test set	1925 reflections (2.03%)	DCC
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	36096	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, FUL, MAN

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	0.43	0/6135	0.85	14/8344 (0.2%)
1	B	0.44	0/6135	0.85	12/8344 (0.1%)
1	C	0.43	0/6135	0.85	11/8344 (0.1%)
1	D	0.43	0/6135	0.85	13/8344 (0.2%)
2	E	0.46	0/2874	1.01	23/3896 (0.6%)
2	F	0.65	2/2874 (0.1%)	1.16	22/3896 (0.6%)
2	G	0.47	0/2874	0.97	17/3896 (0.4%)
2	H	0.47	0/2874	0.97	17/3896 (0.4%)
3	W	0.63	0/54	0.89	0/75
3	X	0.63	0/54	1.30	1/75 (1.3%)
3	Y	0.57	0/54	1.31	1/75 (1.3%)
3	Z	0.56	0/54	0.92	0/75
All	All	0.46	2/36252 (0.0%)	0.91	131/49260 (0.3%)

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
2	E	0	1
2	F	1	1
2	H	0	1
3	X	0	1
3	Y	0	1
All	All	1	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	351	TYR	N-CA	-21.51	1.03	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	350	ALA	C-N	8.11	1.52	1.34

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	350	ALA	O-C-N	-25.49	81.92	122.70
2	F	350	ALA	CA-C-N	17.64	156.01	117.20
2	F	351	TYR	N-CA-CB	16.83	140.90	110.60
2	F	350	ALA	C-N-CA	11.19	149.68	121.70
2	F	296	ASP	CB-CG-OD2	10.62	127.85	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	351	TYR	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	113	GLU	Peptide
2	F	350	ALA	Mainchain
2	H	113	GLU	Peptide
3	X	5	ASP	Peptide
3	Y	3	PRO	Peptide

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	5963	0	5677	59	1
1	B	5963	0	5677	60	0
1	C	5963	0	5676	55	0
1	D	5963	0	5677	68	0
2	E	2809	0	2767	49	1
2	F	2809	0	2767	69	0
2	G	2809	0	2767	65	0
2	H	2809	0	2767	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	51	0	48	3	0
3	X	51	0	48	3	0
3	Y	51	0	48	1	0
3	Z	51	0	48	1	0
4	A	38	0	34	0	0
4	C	38	0	34	0	0
5	A	84	0	75	4	0
5	B	56	0	50	0	0
5	C	84	0	75	1	0
5	D	56	0	50	1	0
6	A	50	0	43	1	0
6	B	50	0	43	0	0
6	C	50	0	43	0	0
6	D	50	0	43	0	0
7	A	42	0	39	0	0
7	B	56	0	52	0	0
7	C	42	0	39	0	0
7	D	56	0	52	0	0
8	B	24	0	22	0	0
8	D	24	0	22	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
All	All	36096	0	34683	468	1

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 468 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:253:ARG:HH22	1:B:253:ARG:HH22	1.09	0.94
2:E:13:GLU:OE1	2:E:294:THR:HG22	1.71	0.90
1:D:340:LEU:HD13	1:D:343:ARG:HD2	1.53	0.89
5:A:850:NAG:O3	5:A:851:NAG:H82	1.74	0.88
2:F:283:PHE:HD2	2:F:288:VAL:HG11	1.40	0.84

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LYS:NZ	2:E:121:GLU:OE2[4_546]	1.77	0.43

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%)	669 (92%)	55 (8%)	2 (0%)	44	80
1	B	726/728 (100%)	672 (93%)	52 (7%)	2 (0%)	44	80
1	C	726/728 (100%)	670 (92%)	55 (8%)	1 (0%)	55	88
1	D	726/728 (100%)	667 (92%)	55 (8%)	4 (1%)	28	70
2	E	350/363 (96%)	309 (88%)	34 (10%)	7 (2%)	9	42
2	F	350/363 (96%)	301 (86%)	37 (11%)	12 (3%)	4	26
2	G	350/363 (96%)	306 (87%)	34 (10%)	10 (3%)	5	31
2	H	350/363 (96%)	307 (88%)	36 (10%)	7 (2%)	9	42
3	W	4/9 (44%)	4 (100%)	0	0	100	100
3	X	4/9 (44%)	2 (50%)	2 (50%)	0	100	100
3	Y	4/9 (44%)	2 (50%)	1 (25%)	1 (25%)	0	0
3	Z	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
All	All	4320/4400 (98%)	3912 (91%)	362 (8%)	46 (1%)	17	57

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	THR
1	D	341	VAL
2	E	113	GLU
2	F	351	TYR
2	F	354	PRO

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	653/653 (100%)	592 (91%)	61 (9%)	10	37
1	B	653/653 (100%)	594 (91%)	59 (9%)	11	39
1	C	653/653 (100%)	595 (91%)	58 (9%)	11	39
1	D	653/653 (100%)	590 (90%)	63 (10%)	10	35
2	E	307/315 (98%)	255 (83%)	52 (17%)	2	11
2	F	307/315 (98%)	260 (85%)	47 (15%)	3	15
2	G	307/315 (98%)	253 (82%)	54 (18%)	2	10
2	H	307/315 (98%)	249 (81%)	58 (19%)	2	9
3	W	6/9 (67%)	6 (100%)	0	100	100
3	X	6/9 (67%)	4 (67%)	2 (33%)	0	0
3	Y	6/9 (67%)	5 (83%)	1 (17%)	2	11
3	Z	6/9 (67%)	4 (67%)	2 (33%)	0	0
All	All	3864/3908 (99%)	3407 (88%)	457 (12%)	6	26

5 of 457 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	358	ARG
2	E	98	VAL
2	H	171	LYS
1	D	410	LEU
1	D	658	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	72	GLN
1	C	483	HIS
2	F	210	HIS
1	C	75	ASN

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Mol	Chain	Res	Type
1	C	314	GLN

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 ⓘ

46 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	800	1,4	14,14,15	0.50	0	15,19,21	1.44	2 (13%)
4	NAG	A	801	4	14,14,15	0.52	0	15,19,21	2.71	7 (46%)
4	FUL	A	802	4	9,10,11	0.63	0	13,14,16	2.34	5 (38%)
5	NAG	A	810	1,5	14,14,15	0.56	0	15,19,21	1.93	6 (40%)
5	NAG	A	811	5	14,14,15	0.66	0	15,19,21	1.83	6 (40%)
5	NAG	A	820	1,5	14,14,15	0.59	0	15,19,21	2.23	4 (26%)
5	NAG	A	821	5	14,14,15	0.55	0	15,19,21	1.62	2 (13%)
6	NAG	A	830	1,6	14,14,15	0.75	0	15,19,21	1.77	3 (20%)
6	NAG	A	831	6	14,14,15	0.62	0	15,19,21	1.70	3 (20%)
6	BMA	A	832	6	11,11,12	0.70	0	13,15,17	2.39	3 (23%)
6	MAN	A	833	6	11,11,12	0.65	0	13,15,17	1.95	3 (23%)
5	NAG	A	850	1,5	14,14,15	0.61	0	15,19,21	1.69	3 (20%)
5	NAG	A	851	5	14,14,15	0.75	0	15,19,21	1.77	3 (20%)
8	NAG	B	800	1,8	14,14,15	0.46	0	15,19,21	2.85	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FUL	B	802	8	9,10,11	0.91	0	13,14,16	2.22	5 (38%)
5	NAG	B	820	1,5	14,14,15	0.47	0	15,19,21	2.83	7 (46%)
5	NAG	B	821	5	14,14,15	0.64	0	15,19,21	1.65	4 (26%)
6	NAG	B	830	1,6	14,14,15	0.73	0	15,19,21	2.04	5 (33%)
6	NAG	B	831	6	14,14,15	0.77	1 (7%)	15,19,21	1.25	2 (13%)
6	BMA	B	832	6	11,11,12	0.73	0	13,15,17	2.29	4 (30%)
6	MAN	B	833	6	11,11,12	0.60	0	13,15,17	1.97	2 (15%)
5	NAG	B	850	1,5	14,14,15	0.89	0	15,19,21	2.11	6 (40%)
5	NAG	B	851	5	14,14,15	0.46	0	15,19,21	2.00	1 (6%)
4	NAG	C	800	1,4	14,14,15	0.58	0	15,19,21	1.38	1 (6%)
4	NAG	C	801	4	14,14,15	0.53	0	15,19,21	2.30	4 (26%)
4	FUL	C	802	4	9,10,11	0.66	0	13,14,16	1.83	2 (15%)
5	NAG	C	810	1,5	14,14,15	0.72	0	15,19,21	3.28	5 (33%)
5	NAG	C	811	5	14,14,15	0.49	0	15,19,21	1.69	4 (26%)
5	NAG	C	820	1,5	14,14,15	0.46	0	15,19,21	2.44	5 (33%)
5	NAG	C	821	5	14,14,15	0.56	0	15,19,21	1.92	5 (33%)
6	NAG	C	830	1,6	14,14,15	0.68	0	15,19,21	2.60	6 (40%)
6	NAG	C	831	6	14,14,15	0.66	0	15,19,21	1.23	2 (13%)
6	BMA	C	832	6	11,11,12	0.51	0	13,15,17	1.52	2 (15%)
6	MAN	C	833	6	11,11,12	0.50	0	13,15,17	2.49	6 (46%)
5	NAG	C	850	1,5	14,14,15	0.68	0	15,19,21	2.60	6 (40%)
5	NAG	C	851	5	14,14,15	0.55	0	15,19,21	1.57	3 (20%)
8	NAG	D	800	1,8	14,14,15	0.72	1 (7%)	15,19,21	2.08	6 (40%)
8	FUL	D	802	8	9,10,11	0.95	0	13,14,16	2.81	6 (46%)
5	NAG	D	820	1,5	14,14,15	0.67	0	15,19,21	1.74	4 (26%)
5	NAG	D	821	5	14,14,15	0.74	1 (7%)	15,19,21	1.94	6 (40%)
6	NAG	D	830	1,6	14,14,15	0.66	0	15,19,21	2.90	5 (33%)
6	NAG	D	831	6	14,14,15	0.58	0	15,19,21	1.48	2 (13%)
6	BMA	D	832	6	11,11,12	0.58	0	13,15,17	2.23	5 (38%)
6	MAN	D	833	6	11,11,12	0.67	0	13,15,17	2.04	4 (30%)
5	NAG	D	850	1,5	14,14,15	0.56	0	15,19,21	2.64	5 (33%)
5	NAG	D	851	5	14,14,15	0.66	0	15,19,21	1.93	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
4	NAG	A	800	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	801	4	-	0/6/23/26	0/1/1/1
4	FUL	A	802	4	-	0/0/17/20	0/1/1/1
5	NAG	A	810	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	811	5	-	0/6/23/26	0/1/1/1
5	NAG	A	820	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	821	5	-	0/6/23/26	0/1/1/1
6	NAG	A	830	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	831	6	-	0/6/23/26	0/1/1/1
6	BMA	A	832	6	-	0/2/19/22	0/1/1/1
6	MAN	A	833	6	-	0/2/19/22	0/1/1/1
5	NAG	A	850	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	851	5	-	0/6/23/26	0/1/1/1
8	NAG	B	800	1,8	-	0/6/23/26	0/1/1/1
8	FUL	B	802	8	-	0/0/17/20	0/1/1/1
5	NAG	B	820	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	821	5	-	0/6/23/26	0/1/1/1
6	NAG	B	830	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	831	6	-	0/6/23/26	0/1/1/1
6	BMA	B	832	6	-	0/2/19/22	0/1/1/1
6	MAN	B	833	6	-	0/2/19/22	0/1/1/1
5	NAG	B	850	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	851	5	-	0/6/23/26	0/1/1/1
4	NAG	C	800	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	801	4	-	0/6/23/26	0/1/1/1
4	FUL	C	802	4	-	0/0/17/20	0/1/1/1
5	NAG	C	810	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	811	5	-	0/6/23/26	0/1/1/1
5	NAG	C	820	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	821	5	-	0/6/23/26	0/1/1/1
6	NAG	C	830	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	831	6	-	0/6/23/26	0/1/1/1
6	BMA	C	832	6	-	0/2/19/22	0/1/1/1
6	MAN	C	833	6	-	0/2/19/22	1/1/1/1
5	NAG	C	850	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	851	5	-	0/6/23/26	0/1/1/1
8	NAG	D	800	1,8	-	2/6/23/26	0/1/1/1
8	FUL	D	802	8	-	0/0/17/20	0/1/1/1
5	NAG	D	820	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	821	5	-	0/6/23/26	0/1/1/1
6	NAG	D	830	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	831	6	-	0/6/23/26	0/1/1/1
6	BMA	D	832	6	-	0/2/19/22	0/1/1/1
6	MAN	D	833	6	-	0/2/19/22	0/1/1/1
5	NAG	D	850	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	851	5	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	831	NAG	O5-C1	-2.06	1.40	1.43
5	D	821	NAG	C1-C2	2.06	1.55	1.52
8	D	800	NAG	C1-C2	2.17	1.55	1.52

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	830	NAG	C1-C2-N2	-8.78	95.49	110.49
4	A	801	NAG	O5-C1-C2	-6.84	101.96	111.47
4	A	802	FUL	C1-C2-C3	-6.41	101.52	109.65
6	B	833	MAN	O5-C1-C2	-5.33	102.44	110.79
8	D	802	FUL	C1-C2-C3	-5.30	102.93	109.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	851	NAG	O7-C7-N2-C2
8	D	800	NAG	C8-C7-N2-C2
8	D	800	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	833	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	830	NAG	1	0
5	A	850	NAG	4	0
5	A	851	NAG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	811	NAG	1	0
5	D	821	NAG	1	0

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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$
7	NAG	A	840	1	14,14,15	0.90	1 (7%)	15,19,21	2.74	5 (33%)
7	NAG	A	860	1	14,14,15	0.78	1 (7%)	15,19,21	2.34	6 (40%)
7	NAG	A	870	1	14,14,15	0.50	0	15,19,21	2.25	3 (20%)
7	NAG	B	810	1	14,14,15	0.68	0	15,19,21	1.99	5 (33%)
7	NAG	B	840	1	14,14,15	0.65	0	15,19,21	3.11	6 (40%)
7	NAG	B	860	1	14,14,15	0.70	0	15,19,21	2.19	6 (40%)
7	NAG	B	870	1	14,14,15	0.44	0	15,19,21	2.03	3 (20%)
7	NAG	C	840	1	14,14,15	0.79	1 (7%)	15,19,21	1.66	5 (33%)
7	NAG	C	860	1	14,14,15	0.89	0	15,19,21	3.57	6 (40%)
7	NAG	C	870	1	14,14,15	0.51	0	15,19,21	1.53	3 (20%)
7	NAG	D	810	1	14,14,15	0.67	0	15,19,21	2.43	6 (40%)
7	NAG	D	840	1	14,14,15	0.88	1 (7%)	15,19,21	3.10	6 (40%)
7	NAG	D	860	1	14,14,15	0.64	0	15,19,21	2.54	7 (46%)
7	NAG	D	870	1	14,14,15	0.64	0	15,19,21	1.91	6 (40%)

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
7	NAG	A	840	1	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	860	1	-	0/6/23/26	0/1/1/1
7	NAG	A	870	1	-	0/6/23/26	0/1/1/1
7	NAG	B	810	1	-	0/6/23/26	0/1/1/1
7	NAG	B	840	1	-	0/6/23/26	0/1/1/1
7	NAG	B	860	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	B	870	1	-	0/6/23/26	0/1/1/1
7	NAG	C	840	1	-	0/6/23/26	0/1/1/1
7	NAG	C	860	1	-	0/6/23/26	0/1/1/1
7	NAG	C	870	1	-	0/6/23/26	0/1/1/1
7	NAG	D	810	1	-	0/6/23/26	0/1/1/1
7	NAG	D	840	1	-	1/6/23/26	0/1/1/1
7	NAG	D	860	1	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	D	870	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	840	NAG	C1-C2	2.05	1.55	1.52
7	A	860	NAG	C1-C2	2.06	1.55	1.52
7	C	840	NAG	C1-C2	2.11	1.55	1.52
7	A	840	NAG	C1-C2	2.65	1.56	1.52

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	840	NAG	O3-C3-C4	-4.65	100.24	110.36
7	A	840	NAG	O5-C1-C2	-4.38	105.38	111.47
7	B	840	NAG	O3-C3-C4	-3.64	102.44	110.36
7	B	860	NAG	O7-C7-C8	-3.54	115.62	122.06
7	B	810	NAG	C6-C5-C4	-3.52	104.78	113.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	860	NAG	C1
7	D	860	NAG	C1
7	A	840	NAG	C5

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	860	NAG	O7-C7-N2-C2
7	D	840	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	728/728 (100%)	-0.35	0 100 100	38, 57, 86, 106	0
1	B	728/728 (100%)	-0.32	1 (0%) 95 94	36, 57, 86, 106	0
1	C	728/728 (100%)	-0.41	2 (0%) 93 92	38, 57, 86, 106	0
1	D	728/728 (100%)	-0.42	2 (0%) 93 92	38, 58, 87, 106	0
2	E	352/363 (96%)	0.19	20 (5%) 24 13	40, 82, 90, 93	0
2	F	352/363 (96%)	0.19	11 (3%) 49 32	67, 83, 91, 100	0
2	G	352/363 (96%)	0.19	12 (3%) 46 29	71, 84, 92, 95	0
2	H	352/363 (96%)	0.21	10 (2%) 53 37	65, 83, 91, 104	0
3	W	6/9 (66%)	0.65	1 (16%) 2 1	72, 82, 94, 95	0
3	X	6/9 (66%)	0.86	1 (16%) 2 1	64, 73, 82, 85	0
3	Y	6/9 (66%)	0.92	2 (33%) 0 0	84, 92, 99, 100	0
3	Z	6/9 (66%)	0.93	2 (33%) 0 0	86, 92, 99, 100	0
All	All	4344/4400 (98%)	-0.18	64 (1%) 74 60	36, 67, 90, 106	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	354	PRO	3.9
2	E	17	HIS	3.7
2	E	15	HIS	3.7
2	E	16	VAL	3.7
2	E	293	ASN	3.7

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

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(Å ²)	Q<0.9
5	NAG	A	850	14/15	0.87	0.30	5.77	73,76,80,84	0
5	NAG	D	850	14/15	0.88	0.27	4.10	75,80,82,83	0
4	NAG	A	800	14/15	0.89	0.29	3.15	92,95,99,100	0
5	NAG	B	850	14/15	0.88	0.29	3.13	75,82,86,86	0
5	NAG	B	821	14/15	0.86	0.33	2.97	67,76,78,81	0
5	NAG	C	850	14/15	0.89	0.26	2.37	71,75,78,79	0
5	NAG	D	821	14/15	0.85	0.38	2.20	84,87,89,90	0
5	NAG	C	821	14/15	0.89	0.31	1.88	91,93,94,94	0
5	NAG	A	821	14/15	0.86	0.33	1.78	82,86,87,87	0
5	NAG	C	810	14/15	0.81	0.33	1.74	91,96,99,104	0
5	NAG	A	810	14/15	0.87	0.25	1.45	77,82,85,90	0
5	NAG	A	820	14/15	0.93	0.24	1.16	77,81,83,84	0
6	NAG	D	831	14/15	0.94	0.24	0.96	68,74,79,83	0
8	NAG	B	800	14/15	0.81	0.25	0.65	80,86,88,89	0
6	NAG	D	830	14/15	0.94	0.18	-0.01	55,60,62,67	0
6	NAG	A	831	14/15	0.95	0.20	-0.12	58,60,63,68	0
4	NAG	C	800	14/15	0.92	0.26	-0.13	99,102,105,108	0
6	NAG	B	831	14/15	0.95	0.23	-0.14	42,45,51,52	0
8	NAG	D	800	14/15	0.88	0.21	-0.78	100,102,103,103	0
6	NAG	A	830	14/15	0.96	0.13	-1.06	44,47,52,54	0
6	NAG	B	830	14/15	0.96	0.13	-1.51	38,39,42,43	0
6	NAG	C	830	14/15	0.96	0.12	-1.67	46,52,58,61	0
5	NAG	A	851	14/15	0.79	0.42	-	86,88,90,90	0
4	FUL	A	802	10/11	0.82	0.32	-	98,99,99,100	0
5	NAG	B	820	14/15	0.94	0.30	-	70,71,72,74	0
6	BMA	C	832	11/12	0.91	0.26	-	85,88,89,90	0
6	MAN	A	833	11/12	0.89	0.31	-	82,84,85,85	0
8	FUL	D	802	10/11	0.85	0.29	-	107,109,110,111	0
6	MAN	B	833	11/12	0.89	0.17	-	68,69,72,73	0
4	FUL	C	802	10/11	0.85	0.34	-	106,106,107,107	0
5	NAG	C	820	14/15	0.93	0.32	-	79,83,85,88	0
5	NAG	C	851	14/15	0.76	0.31	-	99,102,106,107	0
5	NAG	B	851	14/15	0.90	0.32	-	87,88,89,89	0
6	BMA	D	832	11/12	0.89	0.21	-	84,87,89,92	0
5	NAG	D	820	14/15	0.89	0.29	-	78,82,83,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	801	14/15	0.80	0.36	-	97,102,103,104	0
5	NAG	C	811	14/15	0.81	0.43	-	106,107,108,109	0
5	NAG	A	811	14/15	0.81	0.36	-	92,93,96,96	0
6	MAN	D	833	11/12	0.84	0.29	-	91,93,93,94	0
6	MAN	C	833	11/12	0.90	0.23	-	91,92,94,95	0
6	NAG	C	831	14/15	0.91	0.20	-	66,69,74,80	0
4	NAG	C	801	14/15	0.73	0.41	-	110,111,111,112	0
6	BMA	A	832	11/12	0.84	0.22	-	74,76,77,79	0
6	BMA	B	832	11/12	0.93	0.16	-	57,60,61,64	0
5	NAG	D	851	14/15	0.80	0.37	-	98,99,100,101	0
8	FUL	B	802	10/11	0.85	0.37	-	78,83,83,83	0

6.4 Ligands [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
7	NAG	A	860	14/15	0.72	0.44	7.67	89,92,96,97	0
7	NAG	B	860	14/15	0.80	0.38	6.38	84,90,93,93	0
7	NAG	C	860	14/15	0.81	0.36	3.06	92,94,95,96	0
7	NAG	D	860	14/15	0.78	0.33	2.30	87,89,90,91	0
7	NAG	D	840	14/15	0.88	0.19	0.18	64,67,69,69	0
9	ZN	F	501	1/1	0.86	0.24	-1.12	83,83,83,83	0
7	NAG	B	840	14/15	0.87	0.17	-1.22	61,64,66,67	0
9	ZN	G	501	1/1	0.95	0.23	-1.46	85,85,85,85	0
9	ZN	H	501	1/1	0.95	0.20	-1.64	83,83,83,83	0
9	ZN	E	501	1/1	0.97	0.34	-1.73	66,66,66,66	0
7	NAG	D	870	14/15	0.83	0.29	-	101,103,104,104	0
7	NAG	D	810	14/15	0.84	0.29	-	90,94,95,96	0
7	NAG	C	840	14/15	0.88	0.31	-	70,72,76,76	0
7	NAG	A	870	14/15	0.91	0.24	-	93,97,99,99	0
7	NAG	B	870	14/15	0.85	0.23	-	98,102,103,103	0
7	NAG	C	870	14/15	0.79	0.32	-	101,104,106,106	0
7	NAG	A	840	14/15	0.89	0.22	-	69,71,72,72	0
7	NAG	B	810	14/15	0.84	0.24	-	74,82,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.