



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XFD
Title : Structure of a human A-type Potassium Channel Accelerating factor DPPX,
a member of the dipeptidyl aminopeptidase family
Authors : Strop, P.; Bankovich, A.J.; Hansen, K.C.; Garcia, K.C.; Brunger, A.T.
Deposited on : 2004-09-14
Resolution : 3.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

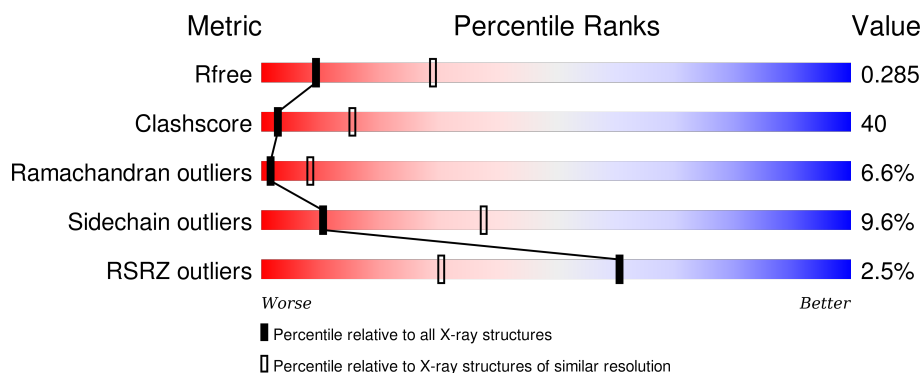
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	723	<div> <div>2%</div> <div>43%</div> <div>46%</div> <div>11%</div> </div>
1	B	723	<div> <div>3%</div> <div>44%</div> <div>44%</div> <div>11%</div> </div>
1	C	723	<div> <div>2%</div> <div>42%</div> <div>46%</div> <div>11%</div> </div>
1	D	723	<div> <div>2%</div> <div>43%</div> <div>45%</div> <div>11%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDG	A	1404	-	-	X	-
2	NAG	A	2404	-	-	X	-
4	BMA	A	3813	-	-	X	-
9	MAN	D	4404	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 24224 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 aminopeptidase-like protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5837	3718	990	1105	24			
1	B	723	Total	C	N	O	S	0	0	0
			5837	3718	990	1105	24			
1	C	723	Total	C	N	O	S	0	0	0
			5837	3718	990	1105	24			
1	D	723	Total	C	N	O	S	0	0	0
			5837	3718	990	1105	24			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

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

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

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

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

- 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	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		

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

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

- 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		

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

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

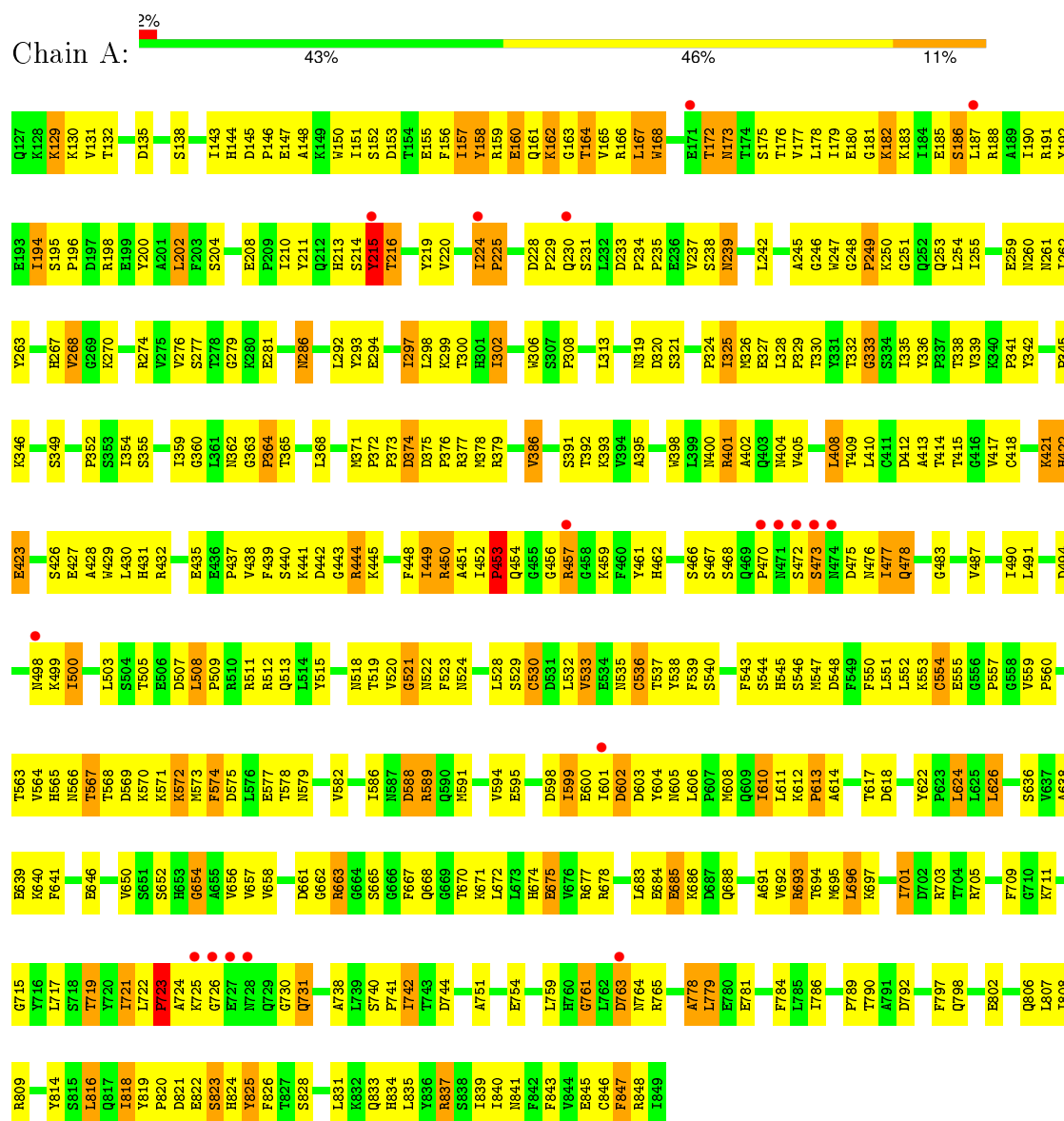
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	13	Total	O	0	0
			13	13		
10	B	14	Total	O	0	0
			14	14		
10	C	14	Total	O	0	0
			14	14		
10	D	10	Total	O	0	0
			10	10		

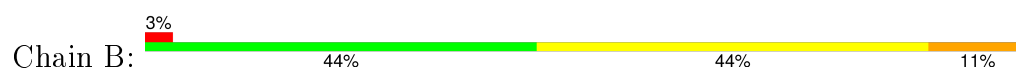
3 Residue-property plots

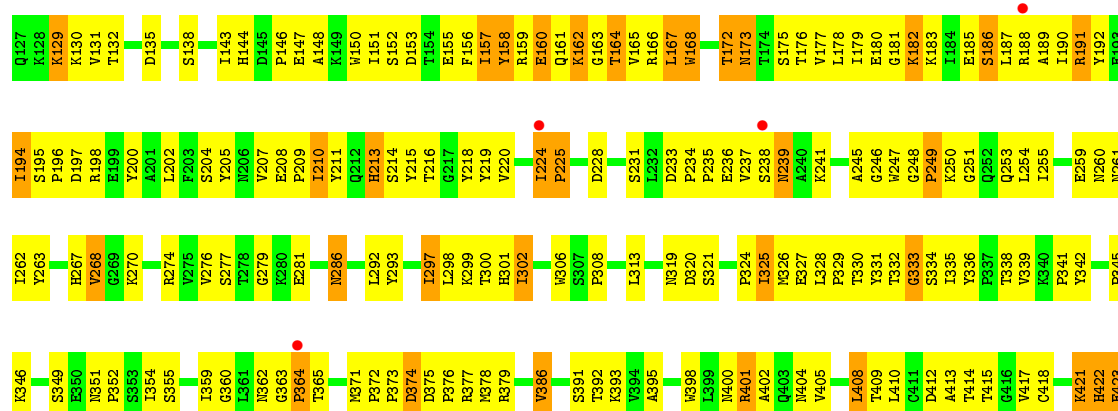
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

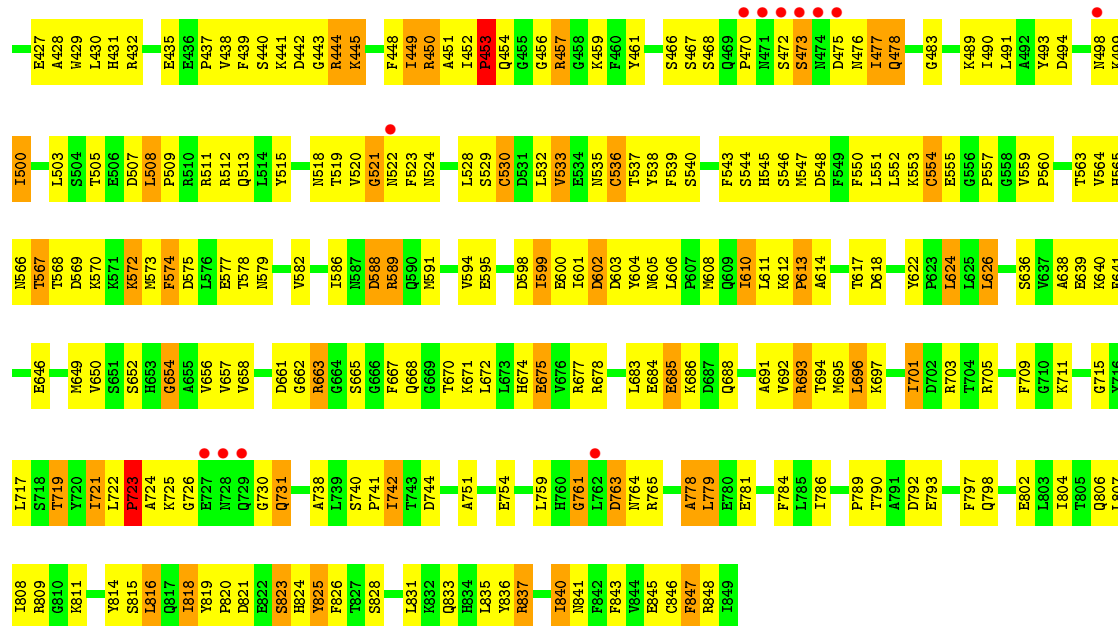
• Molecule 1: Dipeptidyl aminopeptidase-like protein 6



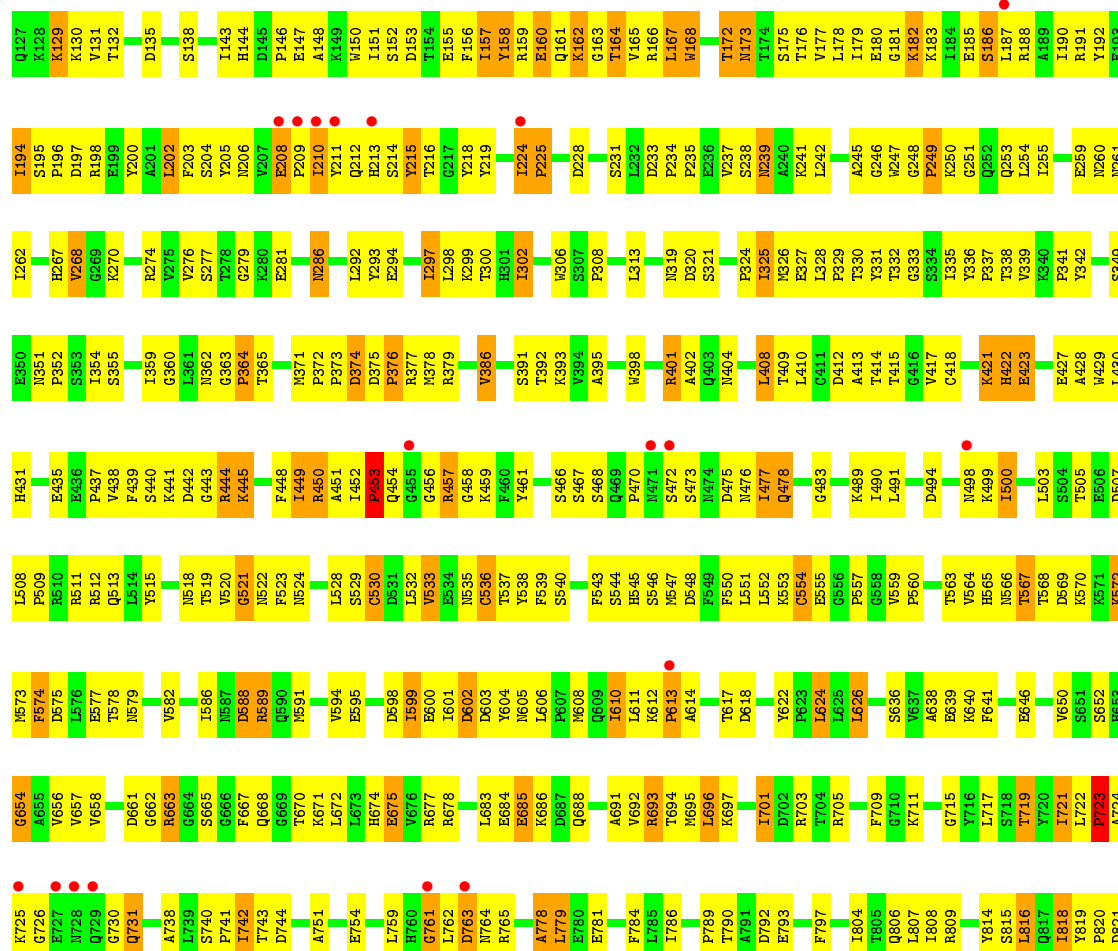
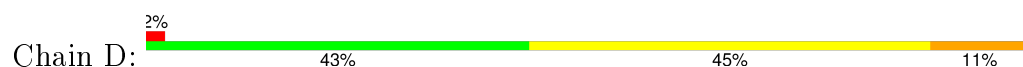
• Molecule 1: Dipeptidyl aminopeptidase-like protein 6







• Molecule 1: Dipeptidyl aminopeptidase-like protein 6



B822	S823	B824	B825	F826	T827	S828
B831	T832	Q833	B834	L835	T836	B837
B840	B841	F842	F843	T844	B845	C846
F847	B848	T849				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.98Å 170.23Å 159.32Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 24.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.6 (15.00-3.00) 77.0 (24.81-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.280 0.255 , 0.285	Depositor DCC
R_{free} test set	3338 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	70.9	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 76240 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24224	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, NDG, 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	0.47	0/5987	0.68	2/8118 (0.0%)
1	B	0.47	0/5987	0.70	3/8118 (0.0%)
1	C	0.51	5/5987 (0.1%)	0.72	8/8118 (0.1%)
1	D	0.46	0/5987	0.68	2/8118 (0.0%)
All	All	0.48	5/23948 (0.0%)	0.70	15/32472 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	840	ILE	CB-CG2	-8.70	1.25	1.52
1	C	191	ARG	CZ-NH2	-8.69	1.21	1.33
1	C	191	ARG	NE-CZ	-8.02	1.22	1.33
1	C	191	ARG	CD-NE	-7.97	1.32	1.46
1	C	191	ARG	CG-CD	-5.22	1.38	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	ARG	NE-CZ-NH2	-15.02	112.79	120.30
1	C	840	ILE	CG1-CB-CG2	-9.11	91.37	111.40
1	C	191	ARG	CD-NE-CZ	-7.57	113.01	123.60
1	C	191	ARG	NH1-CZ-NH2	7.35	127.48	119.40
1	B	212	GLN	N-CA-C	-6.72	92.85	111.00

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	5837	0	5677	467	1
1	B	5837	0	5678	469	1
1	C	5837	0	5679	482	1
1	D	5837	0	5679	465	1
2	A	117	0	102	13	0
2	B	39	0	34	2	0
2	C	39	0	34	1	0
2	D	78	0	68	6	0
3	A	50	0	43	2	0
4	A	50	0	43	10	0
5	A	28	0	25	4	0
5	B	56	0	50	5	0
5	C	56	0	50	5	0
6	B	39	0	34	6	0
6	C	39	0	34	3	0
6	D	39	0	34	4	0
7	B	39	0	34	3	0
7	C	39	0	34	3	0
7	D	39	0	34	5	0
8	B	28	0	25	3	0
9	D	50	0	43	9	0
10	A	13	0	0	2	0
10	B	14	0	0	6	0
10	C	14	0	0	2	0
10	D	10	0	0	2	0
All	All	24224	0	23434	1903	2

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 40.

The worst 5 of 1903 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:D:617:THR:HG22	1:D:618:ASP:H	1.01	1.17
1:A:498:ASN:HA	1:A:519:THR:HG22	1.31	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:ASN:HA	1:C:519:THR:HG22	1.32	1.10
1:D:498:ASN:HA	1:D:519:THR:HG22	1.33	1.09
1:B:617:THR:HG22	1:B:618:ASP:H	1.07	1.09

All (2) 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:C:473:SER:OG	1:D:362:ASN:OD1[2_546]	2.13	0.07
1:A:473:SER:OG	1:B:362:ASN:OD1[2_655]	2.17	0.03

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	721/723 (100%)	578 (80%)	97 (14%)	46 (6%)	2	9
1	B	721/723 (100%)	575 (80%)	98 (14%)	48 (7%)	1	8
1	C	721/723 (100%)	579 (80%)	95 (13%)	47 (6%)	1	8
1	D	721/723 (100%)	577 (80%)	94 (13%)	50 (7%)	1	7
All	All	2884/2892 (100%)	2309 (80%)	384 (13%)	191 (7%)	1	8

5 of 191 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	160	GLU
1	A	162	LYS
1	A	173	ASN
1	A	472	SER

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	643/643 (100%)	581 (90%)	62 (10%)	10	38
1	B	643/643 (100%)	582 (90%)	61 (10%)	11	38
1	C	643/643 (100%)	582 (90%)	61 (10%)	11	38
1	D	643/643 (100%)	580 (90%)	63 (10%)	10	36
All	All	2572/2572 (100%)	2325 (90%)	247 (10%)	10	38

5 of 247 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	723	PRO
1	C	325	ILE
1	D	675	GLU
1	B	790	THR
1	C	164	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	HIS
1	B	422	HIS
1	C	351	ASN
1	C	422	HIS
1	D	422	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 ⓘ

63 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	NDG	A	1173	1,3	14,14,15	0.82	1 (7%)	15,19,21	0.96	1 (6%)
2	NDG	A	1319	1,2	14,14,15	0.59	0	15,19,21	1.11	1 (6%)
2	NDG	A	1404	1,2	14,14,15	0.50	0	15,19,21	0.96	1 (6%)
2	NDG	A	1535	1,2	14,14,15	0.86	1 (7%)	15,19,21	0.98	1 (6%)
5	NDG	A	1566	1,5	14,14,15	1.55	3 (21%)	15,19,21	1.70	5 (33%)
4	NAG	A	1813	1,4	14,14,15	0.48	0	15,19,21	0.67	0
3	NDG	A	2173	3	14,14,15	0.82	0	15,19,21	1.25	2 (13%)
2	NAG	A	2319	2	14,14,15	0.59	0	15,19,21	0.78	1 (6%)
2	NAG	A	2404	2	14,14,15	0.87	0	15,19,21	1.45	3 (20%)
2	NAG	A	2535	2	14,14,15	0.55	0	15,19,21	0.69	0
5	NAG	A	2566	5	14,14,15	1.90	3 (21%)	15,19,21	1.31	2 (13%)
4	NAG	A	2813	4	14,14,15	0.58	0	15,19,21	1.03	1 (6%)
3	MAN	A	3173	3	11,11,12	0.83	0	14,15,17	1.07	2 (14%)
2	BMA	A	3319	2	11,11,12	0.61	0	14,15,17	0.33	0
2	BMA	A	3404	2	11,11,12	0.58	0	14,15,17	0.63	0
2	BMA	A	3535	2	11,11,12	0.45	0	14,15,17	0.31	0
4	BMA	A	3813	4	11,11,12	1.17	2 (18%)	14,15,17	1.69	1 (7%)
3	BMA	A	4173	3	11,11,12	0.72	0	14,15,17	1.29	1 (7%)
4	MAN	A	4813	4	11,11,12	0.89	1 (9%)	14,15,17	1.15	1 (7%)
6	NDG	B	1173	1,6	14,14,15	0.83	1 (7%)	15,19,21	1.16	1 (6%)
2	NDG	B	1319	1,2	14,14,15	0.84	1 (7%)	15,19,21	1.26	1 (6%)
5	NDG	B	1404	1,5	14,14,15	0.58	0	15,19,21	1.38	2 (13%)
5	NDG	B	1535	1,5	14,14,15	0.92	1 (7%)	15,19,21	1.03	1 (6%)
8	NAG	B	1566	1,8	14,14,15	1.14	1 (7%)	15,19,21	1.49	3 (20%)
7	NAG	B	1813	1,7	14,14,15	0.49	0	15,19,21	0.62	0
6	NDG	B	2173	6	14,14,15	0.66	0	15,19,21	1.57	3 (20%)
2	NAG	B	2319	2	14,14,15	0.68	0	15,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	2404	5	14,14,15	0.57	0	15,19,21	0.79	1 (6%)
5	NAG	B	2535	5	14,14,15	0.64	0	15,19,21	0.77	1 (6%)
8	NAG	B	2566	8	14,14,15	0.68	0	15,19,21	0.77	1 (6%)
7	NAG	B	2813	7	14,14,15	0.67	0	15,19,21	1.50	2 (13%)
6	MAN	B	3173	6	11,11,12	0.69	0	14,15,17	0.96	1 (7%)
2	BMA	B	3319	2	11,11,12	0.55	0	14,15,17	0.33	0
7	BMA	B	3813	7	11,11,12	0.55	0	14,15,17	0.63	0
6	NDG	C	1173	1,6	14,14,15	0.70	0	15,19,21	1.28	3 (20%)
2	NDG	C	1319	1,2	14,14,15	0.80	1 (7%)	15,19,21	1.18	1 (6%)
5	NDG	C	1404	1,5	14,14,15	0.57	0	15,19,21	1.01	1 (6%)
5	NDG	C	1535	1,5	14,14,15	0.90	1 (7%)	15,19,21	0.92	0
7	NAG	C	1813	1,7	14,14,15	0.63	0	15,19,21	0.59	0
6	NDG	C	2173	6	14,14,15	0.65	0	15,19,21	1.19	2 (13%)
2	NAG	C	2319	2	14,14,15	0.92	1 (7%)	15,19,21	0.93	0
5	NAG	C	2404	5	14,14,15	0.54	0	15,19,21	0.98	1 (6%)
5	NAG	C	2535	5	14,14,15	0.56	0	15,19,21	0.68	0
7	NAG	C	2813	7	14,14,15	0.63	0	15,19,21	1.44	2 (13%)
6	MAN	C	3173	6	11,11,12	0.65	0	14,15,17	0.92	1 (7%)
2	BMA	C	3319	2	11,11,12	0.57	0	14,15,17	0.49	0
7	BMA	C	3813	7	11,11,12	0.54	0	14,15,17	0.36	0
6	NDG	D	1173	1,6	14,14,15	0.65	0	15,19,21	1.20	2 (13%)
2	NDG	D	1319	1,2	14,14,15	0.77	1 (7%)	15,19,21	1.58	3 (20%)
9	NDG	D	1404	1,9	14,14,15	0.42	0	15,19,21	1.14	2 (13%)
2	NDG	D	1535	1,2	14,14,15	0.80	1 (7%)	15,19,21	1.10	2 (13%)
7	NAG	D	1813	1,7	14,14,15	0.59	0	15,19,21	0.86	1 (6%)
6	NDG	D	2173	6	14,14,15	0.74	0	15,19,21	1.72	4 (26%)
2	NAG	D	2319	2	14,14,15	0.64	0	15,19,21	0.83	1 (6%)
9	NAG	D	2404	9	14,14,15	0.67	0	15,19,21	1.31	2 (13%)
2	NAG	D	2535	2	14,14,15	0.70	0	15,19,21	0.70	0
7	NAG	D	2813	7	14,14,15	0.74	0	15,19,21	1.43	2 (13%)
6	MAN	D	3173	6	11,11,12	0.60	0	14,15,17	1.00	2 (14%)
2	BMA	D	3319	2	11,11,12	0.54	0	14,15,17	0.27	0
9	MAN	D	3404	9	11,11,12	0.93	0	14,15,17	2.75	5 (35%)
2	BMA	D	3535	2	11,11,12	0.51	0	14,15,17	0.29	0
7	BMA	D	3813	7	11,11,12	0.54	0	14,15,17	0.36	0
9	MAN	D	4404	9	11,11,12	0.93	1 (9%)	14,15,17	2.17	3 (21%)

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	NDG	A	1173	1,3	-	0/6/23/26	0/1/1/1
2	NDG	A	1319	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	1404	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	1535	1,2	-	0/6/23/26	0/1/1/1
5	NDG	A	1566	1,5	-	0/6/23/26	0/1/1/1
4	NAG	A	1813	1,4	-	0/6/23/26	0/1/1/1
3	NDG	A	2173	3	-	0/6/23/26	0/1/1/1
2	NAG	A	2319	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2404	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2535	2	-	0/6/23/26	0/1/1/1
5	NAG	A	2566	5	-	0/6/23/26	0/1/1/1
4	NAG	A	2813	4	-	0/6/23/26	0/1/1/1
3	MAN	A	3173	3	-	0/2/19/22	0/1/1/1
2	BMA	A	3319	2	-	0/2/19/22	0/1/1/1
2	BMA	A	3404	2	-	0/2/19/22	0/1/1/1
2	BMA	A	3535	2	-	0/2/19/22	0/1/1/1
4	BMA	A	3813	4	-	0/2/19/22	0/1/1/1
3	BMA	A	4173	3	-	0/2/19/22	0/1/1/1
4	MAN	A	4813	4	-	0/2/19/22	0/1/1/1
6	NDG	B	1173	1,6	-	0/6/23/26	0/1/1/1
2	NDG	B	1319	1,2	-	0/6/23/26	0/1/1/1
5	NDG	B	1404	1,5	-	0/6/23/26	0/1/1/1
5	NDG	B	1535	1,5	-	0/6/23/26	0/1/1/1
8	NAG	B	1566	1,8	-	1/6/23/26	0/1/1/1
7	NAG	B	1813	1,7	-	0/6/23/26	0/1/1/1
6	NDG	B	2173	6	-	0/6/23/26	0/1/1/1
2	NAG	B	2319	2	-	0/6/23/26	0/1/1/1
5	NAG	B	2404	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2535	5	-	0/6/23/26	0/1/1/1
8	NAG	B	2566	8	-	0/6/23/26	0/1/1/1
7	NAG	B	2813	7	-	0/6/23/26	0/1/1/1
6	MAN	B	3173	6	-	0/2/19/22	0/1/1/1
2	BMA	B	3319	2	-	0/2/19/22	0/1/1/1
7	BMA	B	3813	7	-	0/2/19/22	0/1/1/1
6	NDG	C	1173	1,6	-	0/6/23/26	0/1/1/1
2	NDG	C	1319	1,2	-	0/6/23/26	0/1/1/1
5	NDG	C	1404	1,5	-	0/6/23/26	0/1/1/1
5	NDG	C	1535	1,5	-	0/6/23/26	0/1/1/1
7	NAG	C	1813	1,7	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NDG	C	2173	6	-	0/6/23/26	0/1/1/1
2	NAG	C	2319	2	-	0/6/23/26	0/1/1/1
5	NAG	C	2404	5	-	0/6/23/26	0/1/1/1
5	NAG	C	2535	5	-	1/6/23/26	0/1/1/1
7	NAG	C	2813	7	-	0/6/23/26	0/1/1/1
6	MAN	C	3173	6	-	0/2/19/22	0/1/1/1
2	BMA	C	3319	2	-	0/2/19/22	0/1/1/1
7	BMA	C	3813	7	-	0/2/19/22	0/1/1/1
6	NDG	D	1173	1,6	-	0/6/23/26	0/1/1/1
2	NDG	D	1319	1,2	-	0/6/23/26	0/1/1/1
9	NDG	D	1404	1,9	-	2/6/23/26	0/1/1/1
2	NDG	D	1535	1,2	-	0/6/23/26	0/1/1/1
7	NAG	D	1813	1,7	-	0/6/23/26	0/1/1/1
6	NDG	D	2173	6	-	0/6/23/26	0/1/1/1
2	NAG	D	2319	2	-	0/6/23/26	0/1/1/1
9	NAG	D	2404	9	-	0/6/23/26	0/1/1/1
2	NAG	D	2535	2	-	0/6/23/26	0/1/1/1
7	NAG	D	2813	7	-	0/6/23/26	0/1/1/1
6	MAN	D	3173	6	-	0/2/19/22	0/1/1/1
2	BMA	D	3319	2	-	0/2/19/22	0/1/1/1
9	MAN	D	3404	9	-	0/2/19/22	0/1/1/1
2	BMA	D	3535	2	-	0/2/19/22	0/1/1/1
7	BMA	D	3813	7	-	0/2/19/22	0/1/1/1
9	MAN	D	4404	9	-	0/2/19/22	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3813	BMA	C2-C3	-2.03	1.49	1.52
2	C	1319	NDG	C1-C2	2.14	1.55	1.52
5	A	2566	NAG	O5-C1	2.15	1.47	1.43
6	B	1173	NDG	C1-C2	2.29	1.55	1.52
3	A	1173	NDG	C1-C2	2.31	1.55	1.52

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3813	BMA	C1-C2-C3	-5.62	102.89	109.54
6	D	2173	NDG	C4-C3-C2	-3.95	105.09	111.23
6	D	2173	NDG	C2-N2-C7	-3.88	118.06	123.04
7	B	2813	NAG	C4-C3-C2	-3.87	105.22	111.23
2	D	1319	NDG	C3-C4-C5	-3.79	103.58	110.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2535	NAG	O7-C7-N2-C2
9	D	1404	NDG	C8-C7-N2-C2
8	B	1566	NAG	O7-C7-N2-C2
9	D	1404	NDG	O7-C7-N2-C2

There are no ring outliers.

50 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1173	NDG	1	0
2	A	1404	NDG	10	0
2	A	1535	NDG	2	0
5	A	1566	NDG	4	0
4	A	1813	NAG	3	0
3	A	2173	NDG	1	0
2	A	2319	NAG	1	0
2	A	2404	NAG	8	0
4	A	2813	NAG	5	0
3	A	3173	MAN	1	0
4	A	3813	BMA	7	0
4	A	4813	MAN	3	0
6	B	1173	NDG	5	0
2	B	1319	NDG	1	0
5	B	1404	NDG	1	0
5	B	1535	NDG	3	0
8	B	1566	NAG	2	0
7	B	1813	NAG	2	0
6	B	2173	NDG	5	0
2	B	2319	NAG	2	0
5	B	2404	NAG	1	0
5	B	2535	NAG	1	0
8	B	2566	NAG	2	0
7	B	2813	NAG	1	0
6	B	3173	MAN	1	0
7	B	3813	BMA	1	0
6	C	1173	NDG	3	0
5	C	1404	NDG	4	0
5	C	1535	NDG	1	0
7	C	1813	NAG	1	0
6	C	2173	NDG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2319	NAG	1	0
5	C	2404	NAG	3	0
7	C	2813	NAG	2	0
7	C	3813	BMA	2	0
6	D	1173	NDG	3	0
2	D	1319	NDG	2	0
9	D	1404	NDG	3	0
2	D	1535	NDG	3	0
7	D	1813	NAG	3	0
6	D	2173	NDG	3	0
2	D	2319	NAG	3	0
9	D	2404	NAG	2	0
2	D	2535	NAG	1	0
7	D	2813	NAG	2	0
6	D	3173	MAN	1	0
2	D	3319	BMA	1	0
9	D	3404	MAN	3	0
7	D	3813	BMA	2	0
9	D	4404	MAN	6	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	723/723 (100%)	-0.05	18 (2%) 61 30	35, 72, 107, 161	0
1	B	723/723 (100%)	0.00	21 (2%) 55 26	33, 72, 108, 161	0
1	C	723/723 (100%)	-0.03	16 (2%) 65 35	32, 71, 106, 162	0
1	D	723/723 (100%)	-0.03	18 (2%) 61 30	34, 71, 108, 162	0
All	All	2892/2892 (100%)	-0.02	73 (2%) 61 30	32, 72, 108, 162	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	473	SER	10.7
1	C	471	ASN	8.2
1	D	472	SER	7.6
1	A	474	ASN	7.3
1	C	727	GLU	6.8

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
5	NDG	B	1404	14/15	0.89	0.23	0.92	75,86,97,98	0
5	NDG	A	1566	14/15	0.62	0.29	0.36	118,120,122,123	0
8	NAG	B	1566	14/15	0.80	0.23	0.01	109,120,124,129	0
2	NDG	A	1404	14/15	0.84	0.21	-0.31	98,105,111,117	0
5	NDG	C	1404	14/15	0.87	0.18	-0.34	92,97,102,105	0
3	NDG	A	1173	14/15	0.73	0.21	-0.57	86,91,98,99	0
4	NAG	A	1813	14/15	0.85	0.19	-0.79	77,84,93,100	0
9	NDG	D	1404	14/15	0.83	0.18	-0.83	84,87,95,111	0
7	NAG	D	1813	14/15	0.89	0.20	-0.89	84,88,93,102	0
7	NAG	C	1813	14/15	0.90	0.20	-0.93	87,92,97,104	0
6	NDG	C	1173	14/15	0.89	0.17	-1.03	82,92,94,100	0
7	NAG	B	1813	14/15	0.86	0.19	-1.33	83,87,92,97	0
3	MAN	A	3173	11/12	0.73	0.17	-	103,108,110,111	0
6	NDG	D	2173	14/15	0.81	0.22	-	104,109,110,112	0
5	NAG	B	2404	14/15	0.87	0.20	-	105,111,113,113	0
2	NAG	B	2319	14/15	0.60	0.34	-	107,115,119,123	0
2	NDG	A	1319	14/15	0.92	0.18	-	52,71,76,91	0
2	NAG	A	2535	14/15	0.74	0.23	-	132,137,141,145	0
2	NAG	D	2319	14/15	0.51	0.38	-	106,113,115,120	0
7	NAG	C	2813	14/15	0.83	0.24	-	112,117,123,127	0
2	NAG	A	2404	14/15	0.63	0.25	-	122,126,130,133	0
2	NDG	A	1535	14/15	0.82	0.17	-	111,114,117,126	0
5	NDG	C	1535	14/15	0.75	0.24	-	109,118,121,123	0
2	NDG	B	1319	14/15	0.90	0.18	-	69,84,90,101	0
6	NDG	C	2173	14/15	0.76	0.25	-	102,110,118,119	0
6	NDG	B	2173	14/15	0.87	0.19	-	113,118,125,126	0
3	NDG	A	2173	14/15	0.83	0.21	-	86,94,99,103	0
6	MAN	B	3173	11/12	0.75	0.28	-	129,132,133,134	0
7	BMA	B	3813	11/12	0.58	0.40	-	125,129,131,131	0
5	NAG	C	2404	14/15	0.77	0.24	-	108,111,115,117	0
2	NDG	D	1535	14/15	0.76	0.17	-	113,118,122,129	0
6	NDG	D	1173	14/15	0.89	0.18	-	93,96,100,101	0
2	NDG	C	1319	14/15	0.90	0.20	-	69,77,81,95	0
5	NAG	B	2535	14/15	0.74	0.33	-	134,137,139,140	0
9	NAG	D	2404	14/15	0.62	0.29	-	123,131,134,143	0
8	NAG	B	2566	14/15	0.64	0.42	-	127,137,143,143	0
7	NAG	D	2813	14/15	0.79	0.28	-	109,118,122,130	0
4	NAG	A	2813	14/15	0.83	0.22	-	108,112,120,128	0
6	MAN	C	3173	11/12	0.63	0.24	-	125,127,128,130	0
5	NDG	B	1535	14/15	0.81	0.21	-	119,123,126,131	0
9	MAN	D	4404	11/12	0.73	0.77	-	163,165,166,167	0
7	NAG	B	2813	14/15	0.83	0.16	-	96,104,110,119	0
4	MAN	A	4813	11/12	0.34	0.61	-	146,148,150,150	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BMA	C	3319	11/12	0.24	0.42	-	131,134,136,137	0
7	BMA	D	3813	11/12	0.21	0.38	-	133,137,139,139	0
2	BMA	A	3319	11/12	0.18	0.70	-	131,135,137,137	0
5	NAG	C	2535	14/15	0.77	0.22	-	127,128,129,129	0
2	NAG	A	2319	14/15	0.55	0.38	-	104,111,118,126	0
2	BMA	A	3535	11/12	0.62	0.39	-	150,152,153,153	0
2	BMA	B	3319	11/12	0.55	0.26	-	119,126,128,128	0
9	MAN	D	3404	11/12	0.69	0.43	-	150,154,156,160	0
2	NAG	C	2319	14/15	0.45	0.33	-	103,113,117,124	0
2	BMA	A	3404	11/12	0.62	0.24	-	136,137,138,138	0
6	MAN	D	3173	11/12	0.73	0.22	-	110,113,115,116	0
2	BMA	D	3535	11/12	0.69	0.24	-	144,146,148,148	0
3	BMA	A	4173	11/12	0.69	0.18	-	113,116,118,119	0
4	BMA	A	3813	11/12	0.67	0.39	-	135,138,141,145	0
2	NDG	D	1319	14/15	0.89	0.21	-	72,79,85,97	0
5	NAG	A	2566	14/15	0.63	0.34	-	125,127,129,129	0
7	BMA	C	3813	11/12	0.52	0.22	-	132,135,136,136	0
6	NDG	B	1173	14/15	0.85	0.15	-	98,101,104,109	0
2	BMA	D	3319	11/12	0.59	0.32	-	124,125,128,128	0
2	NAG	D	2535	14/15	0.58	0.36	-	133,135,138,142	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.