WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:48 am GMT

PDB ID	:	5I7U
Title	:	Human DPP4 in complex with a novel tricyclic hetero-cycle inhibitor
Authors	:	Scapin, G.
Deposited on	:	2016-02-18
Resolution	:	1.95 Å(reported)

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
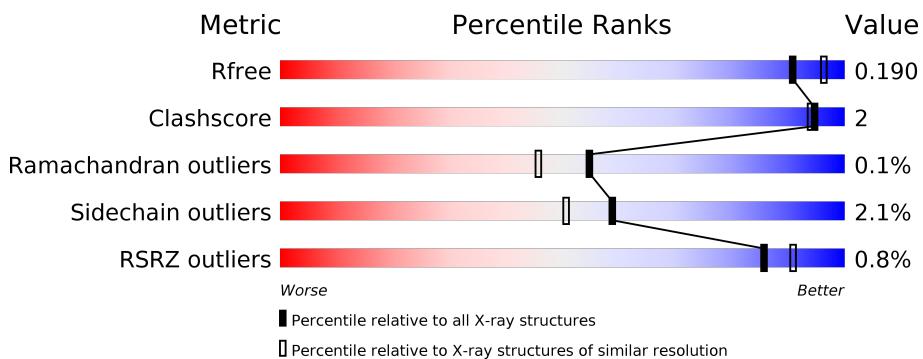
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
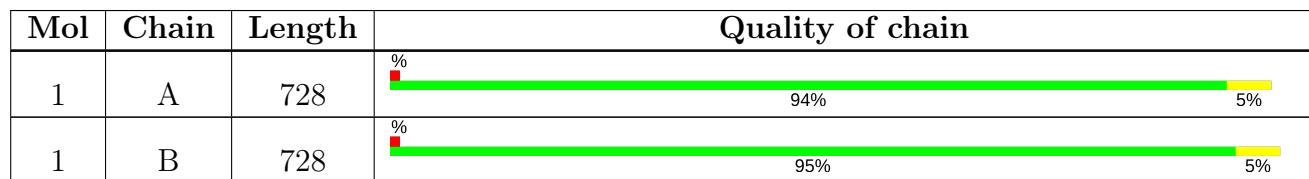
The reported resolution of this entry is 1.95 Å.

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	Percentile Ranks	Value
Rfree		0.190
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		2.1%
RSRZ outliers		0.8%

Worse — *Better*

▌ Percentile relative to all X-ray structures

❑ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	94% 5%
1	B	728	95% 5%

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	NAG	A	801	-	-	-	X
2	NAG	A	805	-	-	-	X
2	NAG	A	806	-	-	-	X
2	NAG	A	810	-	-	-	X
2	NAG	B	801	-	-	-	X
2	NAG	B	803	X	-	-	-
2	NAG	B	805	-	-	-	X
2	NAG	B	811	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14529 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.
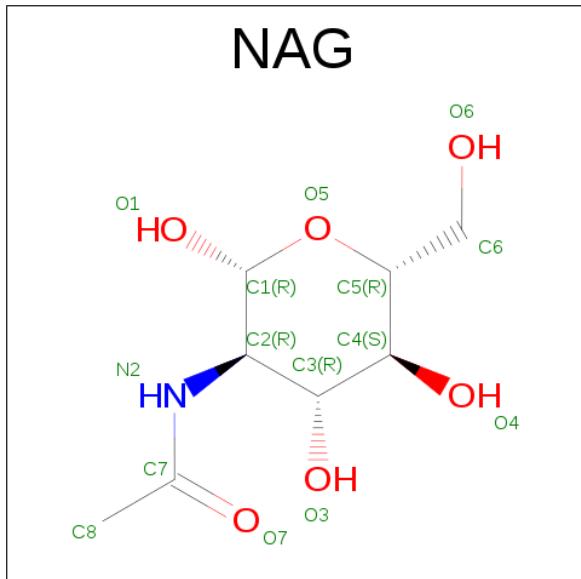
- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total 6004	C 3853	N 991	O 1134	S 26	0	8	0
1	B	728	Total 5992	C 3848	N 983	O 1134	S 27	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	SER	engineered mutation	UNP P27487
B	39	THR	SER	engineered mutation	UNP P27487

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
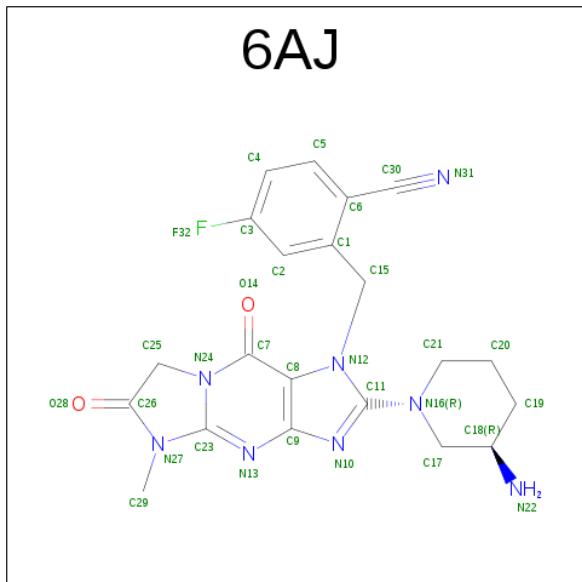
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0

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| 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	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	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	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	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		

- Molecule 3 is 2-({2-[(3R)-3-aminopiperidin-1-yl]-5-methyl-6,9-dioxo-5,6,7,9-tetrahydro-1H
  -imidazo[1,2-a]purin-1-yl}methyl)-4-fluorobenzonitrile (three-letter code: 6AJ) (formula:
  $C_{21}H_{21}FN_8O_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			32	21	1	8	2		
3	B	1	Total	C	F	N	O	0	0
			32	21	1	8	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
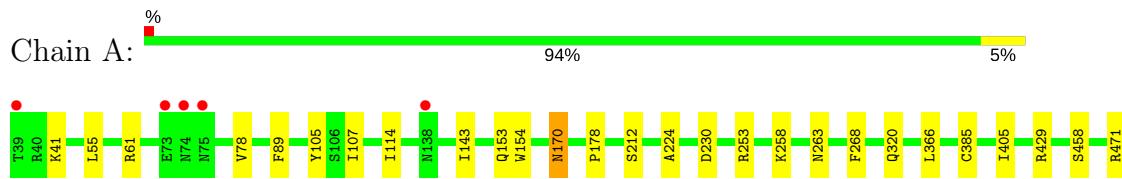
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1102	Total	O	0	0
			1102	1102		
5	B	1058	Total	O	0	0
			1058	1058		
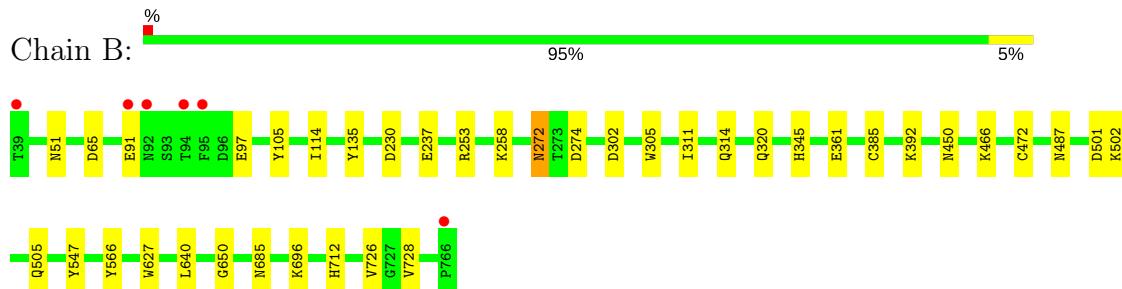
3 Residue-property plots ⓘ

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 4

Chain A:

• Molecule 1: Dipeptidyl peptidase 4

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.55Å 126.55Å 137.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.22 – 1.95 89.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (93.22-1.95) 99.8 (89.89-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 1.95Å)	Xtriage
Refinement program	BUSTER-TNT 2.9.4	Depositor
R, R_{free}	0.154 , 0.187 0.157 , 0.190	Depositor DCC
R_{free} test set	7619 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 6AJ, NA, 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	0.52	0/6206	0.64	0/8438
1	B	0.51	0/6184	0.64	0/8411
All	All	0.51	0/12390	0.64	0/16849

There are no bond length outliers.

There are no bond angle outliers.

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	6004	0	5725	19	0
1	B	5992	0	5718	20	0
2	A	154	0	138	0	0
2	B	154	0	139	0	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
4	A	1	0	0	0	0
5	A	1102	0	0	0	0
5	B	1058	0	0	3	0
All	All	14529	0	11720	37	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 2.

All (37) 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:HH21	1:B:253:ARG:HH21	1.15	0.90
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.71	0.71
1:A:458:SER:OG	1:A:471[B]:ARG:NH1	2.27	0.68
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.94	0.66
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.82	0.61
1:A:471[A]:ARG:HG3	1:A:480:TYR:CE2	2.39	0.57
1:A:258:LYS:NZ	1:A:712:HIS:HD2	2.03	0.57
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.86	0.56
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.90	0.53
1:A:61:ARG:HH22	1:A:107:ILE:H	1.56	0.52
1:B:272:ASN:C	1:B:272:ASN:HD22	2.12	0.52
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.90	0.52
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.75	0.50
1:B:361:GLU:HG3	5:B:1747:HOH:O	2.12	0.50
1:A:78:VAL:HG22	1:A:89:PHE:HB2	1.94	0.49
1:A:143:ILE:HD13	1:A:178:PRO:HB2	1.94	0.49
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.95	0.49
1:B:237[A]:GLU:HG2	1:B:253:ARG:HG2	1.96	0.48
1:B:392:LYS:NZ	5:B:904:HOH:O	2.47	0.48
1:A:154:TRP:CE2	1:A:212[A]:SER:HB3	2.49	0.48
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.12	0.48
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.98	0.47
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.63	0.47
1:A:405:ILE:HG13	1:A:429[A]:ARG:HD2	1.97	0.47
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	1.62	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.98	0.45
1:A:154:TRP:CE2	1:A:212[B]:SER:HB2	2.53	0.44
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.01	0.42
1:A:510:PRO:HD3	1:A:569:SER:HB2	2.01	0.42
1:A:258:LYS:HZ3	1:A:712:HIS:HD2	1.66	0.42
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.56	0.41
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.51	0.41
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.55	0.41
1:B:345:HIS:HD2	5:B:1023:HOH:O	2.04	0.41
1:B:501:ASP:O	1:B:505:GLN:HG2	2.21	0.41
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.21	0.40
1:A:405:ILE:HG13	1:A:429[A]:ARG:CD	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/728 (101%)	713 (97%)	20 (3%)	1 (0%)	55	46
1	B	732/728 (100%)	708 (97%)	23 (3%)	1 (0%)	55	46
All	All	1466/1456 (101%)	1421 (97%)	43 (3%)	2 (0%)	55	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	B	320	GLN

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	661/653 (101%)	648 (98%)	13 (2%)	60	52
1	B	659/653 (101%)	644 (98%)	15 (2%)	56	47
All	All	1320/1306 (101%)	1292 (98%)	28 (2%)	59	50

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	55	LEU
1	A	170	ASN
1	A	230	ASP

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Mol	Chain	Res	Type
1	A	263	ASN
1	A	366	LEU
1	A	385	CYS
1	A	472	CYS
1	A	520	ASN
1	A	521	GLU
1	A	547	TYR
1	A	566	TYR
1	A	627	TRP
1	B	51	ASN
1	B	91	GLU
1	B	97	GLU
1	B	230	ASP
1	B	272	ASN
1	B	385	CYS
1	B	450[A]	ASN
1	B	450[B]	ASN
1	B	472	CYS
1	B	487	ASN
1	B	502	LYS
1	B	547	TYR
1	B	566	TYR
1	B	627	TRP
1	B	685	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	169	ASN
1	A	170	ASN
1	A	263	ASN
1	A	435	GLN
1	A	572	ASN
1	A	694	ASN
1	A	712	HIS
1	B	169	ASN
1	B	272	ASN
1	B	345	HIS
1	B	487	ASN
1	B	572	ASN
1	B	694	ASN

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Mol	Chain	Res	Type
1	B	712	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 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	$\#|Z| > 2$
2	NAG	A	801	1,2	14,14,15	0.95	0	15,19,21	1.55	1 (6%)
2	NAG	A	802	2	14,14,15	1.38	3 (21%)	15,19,21	1.39	3 (20%)
2	NAG	A	803	1,2	14,14,15	1.14	1 (7%)	15,19,21	1.65	4 (26%)
2	NAG	A	804	2	14,14,15	1.46	1 (7%)	15,19,21	3.11	6 (40%)
2	NAG	A	805	1,2	14,14,15	1.51	1 (7%)	15,19,21	1.39	1 (6%)
2	NAG	A	806	2	14,14,15	1.22	2 (14%)	15,19,21	1.89	4 (26%)
2	NAG	A	807	1,2	14,14,15	0.85	0	15,19,21	1.59	2 (13%)
2	NAG	A	808	2	14,14,15	1.58	3 (21%)	15,19,21	1.78	4 (26%)
2	NAG	A	809	1	14,14,15	1.51	1 (7%)	15,19,21	1.13	2 (13%)
2	NAG	A	810	1,2	14,14,15	1.60	4 (28%)	15,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z \rvert > 2$	Counts	RMSZ	$\#\lvert Z \rvert > 2$
2	NAG	A	811	2	14,14,15	1.24	1 (7%)	15,19,21	1.53	3 (20%)
3	6AJ	A	812	-	30,36,36	1.66	9 (30%)	32,54,54	2.88	10 (31%)
2	NAG	B	801	1,2	14,14,15	1.20	1 (7%)	15,19,21	1.28	2 (13%)
2	NAG	B	802	2	14,14,15	2.04	3 (21%)	15,19,21	2.12	3 (20%)
2	NAG	B	803	1	14,14,15	1.34	2 (14%)	15,19,21	1.53	2 (13%)
2	NAG	B	804	1	14,14,15	1.67	3 (21%)	15,19,21	1.11	1 (6%)
2	NAG	B	805	1,2	14,14,15	1.56	2 (14%)	15,19,21	1.42	3 (20%)
2	NAG	B	806	2	14,14,15	1.35	2 (14%)	15,19,21	1.57	3 (20%)
2	NAG	B	807	1,2	14,14,15	1.31	2 (14%)	15,19,21	1.29	2 (13%)
2	NAG	B	808	2	14,14,15	1.41	1 (7%)	15,19,21	0.87	0
2	NAG	B	809	1,2	14,14,15	1.14	1 (7%)	15,19,21	1.40	1 (6%)
2	NAG	B	810	2	14,14,15	1.65	5 (35%)	15,19,21	1.75	3 (20%)
2	NAG	B	811	1	14,14,15	1.63	4 (28%)	15,19,21	1.38	1 (6%)
3	6AJ	B	812	-	30,36,36	1.77	10 (33%)	32,54,54	3.05	13 (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
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	804	2	-	0/6/23/26	0/1/1/1
2	NAG	A	805	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	806	2	-	0/6/23/26	0/1/1/1
2	NAG	A	807	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	808	2	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	811	2	-	0/6/23/26	0/1/1/1
3	6AJ	A	812	-	-	0/6/32/32	0/4/5/5
2	NAG	B	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	802	2	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	806	2	-	0/6/23/26	0/1/1/1

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	807	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	808	2	-	0/6/23/26	0/1/1/1
2	NAG	B	809	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	810	2	-	0/6/23/26	0/1/1/1
2	NAG	B	811	1	-	0/6/23/26	0/1/1/1
3	6AJ	B	812	-	-	0/6/32/32	0/4/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	812	6AJ	C23-N27	-2.37	1.35	1.39
3	B	812	6AJ	F32-C3	-2.04	1.31	1.36
3	B	812	6AJ	C23-N13	-2.03	1.28	1.32
2	A	810	NAG	C4-C3	2.01	1.57	1.52
2	B	810	NAG	C3-C2	2.01	1.56	1.52
2	B	805	NAG	C4-C5	2.02	1.57	1.53
2	A	802	NAG	C3-C2	2.03	1.56	1.52
2	A	810	NAG	C3-C2	2.08	1.57	1.52
3	A	812	6AJ	C5-C6	2.10	1.43	1.40
2	B	803	NAG	C3-C2	2.12	1.57	1.52
2	A	806	NAG	C3-C2	2.15	1.57	1.52
2	B	810	NAG	C4-C5	2.19	1.57	1.53
3	A	812	6AJ	C2-C1	2.19	1.43	1.39
2	A	810	NAG	C4-C5	2.20	1.57	1.53
2	B	811	NAG	C4-C3	2.24	1.58	1.52
3	B	812	6AJ	C4-C3	2.25	1.41	1.37
3	B	812	6AJ	C2-C3	2.25	1.41	1.37
2	B	806	NAG	C4-C3	2.30	1.58	1.52
2	B	810	NAG	C1-C2	2.32	1.55	1.52
2	B	811	NAG	C4-C5	2.34	1.58	1.53
3	A	812	6AJ	C20-C19	2.36	1.59	1.53
2	B	811	NAG	O4-C4	2.37	1.48	1.43
3	B	812	6AJ	C7-C8	2.38	1.45	1.41
3	A	812	6AJ	C19-C18	2.41	1.58	1.51
3	A	812	6AJ	C2-C3	2.41	1.41	1.37
2	B	807	NAG	C4-C5	2.43	1.58	1.53
2	B	804	NAG	C4-C5	2.45	1.58	1.53
3	A	812	6AJ	C18-N22	2.45	1.53	1.47
2	A	808	NAG	C3-C2	2.45	1.57	1.52
2	A	811	NAG	C1-C2	2.49	1.55	1.52
2	A	802	NAG	C4-C5	2.51	1.58	1.53
2	A	802	NAG	C4-C3	2.56	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	808	NAG	C4-C3	2.58	1.58	1.52
2	B	810	NAG	C2-N2	2.62	1.50	1.46
2	A	806	NAG	C1-C2	2.69	1.56	1.52
2	B	801	NAG	C1-C2	2.70	1.56	1.52
2	B	811	NAG	C3-C2	2.74	1.58	1.52
2	B	809	NAG	C1-C2	2.78	1.56	1.52
2	B	810	NAG	C4-C3	2.79	1.59	1.52
2	B	804	NAG	C3-C2	2.82	1.58	1.52
2	B	806	NAG	C1-C2	2.82	1.56	1.52
3	A	812	6AJ	C5-C4	2.83	1.43	1.38
3	B	812	6AJ	C18-N22	2.84	1.54	1.47
3	B	812	6AJ	C5-C4	2.84	1.43	1.38
3	A	812	6AJ	C9-N13	2.87	1.42	1.36
2	B	803	NAG	C1-C2	2.89	1.56	1.52
2	B	802	NAG	C3-C2	2.93	1.58	1.52
2	A	803	NAG	C1-C2	2.98	1.56	1.52
2	B	807	NAG	C1-C2	3.08	1.56	1.52
3	A	812	6AJ	C7-C8	3.11	1.46	1.41
3	B	812	6AJ	C5-C6	3.11	1.45	1.40
2	A	808	NAG	C1-C2	3.13	1.56	1.52
2	B	804	NAG	C1-C2	3.14	1.56	1.52
2	B	808	NAG	C1-C2	3.20	1.56	1.52
2	B	802	NAG	C2-N2	3.26	1.52	1.46
2	A	804	NAG	C1-C2	3.37	1.57	1.52
3	B	812	6AJ	C9-N13	3.56	1.43	1.36
2	A	810	NAG	C1-C2	3.93	1.57	1.52
2	A	809	NAG	C1-C2	3.96	1.57	1.52
2	A	805	NAG	C1-C2	4.45	1.58	1.52
2	B	805	NAG	C1-C2	4.54	1.58	1.52
2	B	802	NAG	C1-C2	5.29	1.59	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	812	6AJ	C8-C7-N24	-12.56	111.80	120.52
3	A	812	6AJ	C8-C7-N24	-11.95	112.22	120.52
2	A	807	NAG	O4-C4-C3	-4.83	99.85	110.36
3	B	812	6AJ	C15-C1-C2	-3.68	113.79	119.69
3	A	812	6AJ	C21-N16-C11	-3.66	113.90	122.07
3	A	812	6AJ	C15-C1-C2	-3.64	113.85	119.69
3	A	812	6AJ	C17-N16-C11	-3.55	114.16	122.07
3	B	812	6AJ	C17-N16-C11	-3.43	114.43	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	812	6AJ	C26-C25-N24	-3.40	98.79	102.04
3	B	812	6AJ	C21-N16-C11	-3.09	115.18	122.07
3	A	812	6AJ	C17-C18-N22	-3.01	104.43	111.32
3	B	812	6AJ	C19-C20-C21	-2.91	107.12	110.96
2	A	802	NAG	O5-C1-C2	-2.91	107.43	111.47
2	A	806	NAG	C8-C7-N2	-2.52	111.55	116.11
2	A	808	NAG	O5-C1-C2	-2.39	108.14	111.47
2	B	805	NAG	O4-C4-C3	-2.28	105.39	110.36
3	B	812	6AJ	C5-C6-C30	-2.25	115.32	119.41
2	B	806	NAG	O3-C3-C2	-2.24	104.58	109.39
2	B	805	NAG	C8-C7-N2	-2.16	112.20	116.11
2	A	803	NAG	O4-C4-C3	-2.14	105.71	110.36
2	B	807	NAG	O4-C4-C5	-2.00	104.24	109.28
2	A	809	NAG	O5-C1-C2	2.02	114.28	111.47
3	A	812	6AJ	C21-N16-C17	2.04	117.04	113.14
2	B	806	NAG	C2-N2-C7	2.06	125.95	122.94
3	B	812	6AJ	O28-C26-N27	2.07	125.47	123.95
3	A	812	6AJ	C1-C15-N12	2.10	116.78	113.31
2	B	803	NAG	O7-C7-N2	2.12	125.99	121.92
2	A	807	NAG	C1-C2-N2	2.15	114.16	110.49
2	B	807	NAG	O7-C7-C8	2.15	125.97	122.06
2	A	806	NAG	C4-C3-C2	2.20	114.24	111.02
2	A	804	NAG	C4-C3-C2	2.30	114.39	111.02
2	B	801	NAG	C4-C3-C2	2.33	114.44	111.02
3	A	812	6AJ	C7-C8-C9	2.36	121.55	119.92
2	A	803	NAG	O5-C1-C2	2.45	114.89	111.47
2	A	805	NAG	O5-C1-C2	2.46	114.90	111.47
2	A	803	NAG	C4-C3-C2	2.47	114.64	111.02
2	A	809	NAG	C1-O5-C5	2.48	115.58	112.17
2	A	802	NAG	C3-C4-C5	2.51	114.64	110.22
2	B	804	NAG	C1-O5-C5	2.54	115.67	112.17
2	B	805	NAG	O5-C1-C2	2.58	115.06	111.47
2	B	810	NAG	C1-C2-N2	2.63	114.98	110.49
2	A	806	NAG	C3-C4-C5	2.64	114.88	110.22
2	A	808	NAG	C2-N2-C7	2.66	126.82	122.94
2	B	801	NAG	O3-C3-C4	2.67	116.17	110.36
2	A	802	NAG	C4-C3-C2	2.72	115.01	111.02
2	A	811	NAG	C2-N2-C7	2.74	126.94	122.94
2	A	804	NAG	C3-C4-C5	2.81	115.17	110.22
2	A	808	NAG	C4-C3-C2	2.81	115.14	111.02
3	B	812	6AJ	C1-C15-N12	2.82	118.00	113.31
2	A	811	NAG	C1-O5-C5	2.88	116.14	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	812	6AJ	O28-C26-C25	3.07	123.72	119.42
2	A	803	NAG	C1-O5-C5	3.07	116.40	112.17
2	A	811	NAG	O5-C1-C2	3.12	115.81	111.47
2	A	801	NAG	C1-O5-C5	3.13	116.48	112.17
2	B	806	NAG	C4-C3-C2	3.19	115.69	111.02
3	B	812	6AJ	C7-C8-C9	3.19	122.13	119.92
3	B	812	6AJ	C1-C6-C30	3.22	123.42	120.24
2	A	804	NAG	C1-C2-N2	3.36	116.22	110.49
2	B	810	NAG	C3-C4-C5	3.42	116.24	110.22
2	B	809	NAG	O3-C3-C4	3.47	117.90	110.36
2	B	810	NAG	C4-C3-C2	3.51	116.16	111.02
2	A	808	NAG	C1-C2-N2	3.55	116.55	110.49
2	B	803	NAG	C2-N2-C7	3.73	128.38	122.94
2	B	802	NAG	C2-N2-C7	3.74	128.40	122.94
3	B	812	6AJ	C15-C1-C6	4.00	125.85	120.45
2	A	804	NAG	C2-N2-C7	4.01	128.79	122.94
3	A	812	6AJ	O28-C26-C25	4.05	125.10	119.42
2	B	811	NAG	C1-O5-C5	4.37	118.19	112.17
2	B	802	NAG	C4-C3-C2	4.41	117.47	111.02
3	A	812	6AJ	C15-C1-C6	4.64	126.71	120.45
2	B	802	NAG	O5-C1-C2	4.85	118.22	111.47
2	A	806	NAG	C1-O5-C5	4.94	118.98	112.17
2	A	804	NAG	O5-C1-C2	5.78	119.51	111.47
2	A	804	NAG	C1-O5-C5	7.77	122.88	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	803	NAG	C1

There are no torsion outliers.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	728/728 (100%)	-0.30	6 (0%)	86	91	12, 21, 48, 71	0
1	B	728/728 (100%)	-0.31	6 (0%)	86	91	13, 22, 48, 74	0
All	All	1456/1456 (100%)	-0.30	12 (0%)	86	91	12, 22, 48, 74	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	7.2
1	A	766	PRO	3.9
1	B	39	THR	3.6
1	B	766	PRO	3.5
1	A	74	ASN	3.4
1	A	73	GLU	2.7
1	B	91	GLU	2.4
1	B	95	PHE	2.3
1	B	92	ASN	2.3
1	A	138	ASN	2.2
1	B	94	THR	2.0
1	A	75	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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(Å^2)	Q<0.9
2	NAG	A	810	14/15	0.85	0.21	6.71	45,49,51,52	0
2	NAG	A	806	14/15	0.76	0.19	6.54	55,59,61,62	0
2	NAG	B	805	14/15	0.94	0.11	5.00	33,37,39,41	0
2	NAG	B	811	14/15	0.82	0.18	4.80	38,42,45,46	0
2	NAG	A	805	14/15	0.91	0.14	3.82	36,40,43,44	0
2	NAG	A	801	14/15	0.82	0.16	3.35	47,50,54,55	0
2	NAG	B	801	14/15	0.81	0.16	2.21	52,56,59,59	0
2	NAG	B	809	14/15	0.92	0.11	1.70	28,32,36,37	0
2	NAG	A	807	14/15	0.94	0.10	1.42	31,35,38,39	0
2	NAG	B	806	14/15	0.88	0.14	1.31	47,51,54,54	0
2	NAG	B	807	14/15	0.95	0.09	0.34	25,28,32,33	0
3	6AJ	B	812	32/32	0.98	0.08	-0.87	12,16,24,27	0
3	6AJ	A	812	32/32	0.97	0.07	-1.15	11,15,26,31	0
4	NA	A	813	1/1	0.99	0.06	-2.18	21,21,21,21	0
2	NAG	A	811	14/15	0.67	0.34	-	77,81,83,83	0
2	NAG	B	802	14/15	0.44	0.30	-	76,79,82,82	0
2	NAG	B	810	14/15	0.61	0.22	-	52,56,58,58	0
2	NAG	B	804	14/15	0.75	0.20	-	55,59,62,62	0
2	NAG	A	802	14/15	0.55	0.29	-	69,73,75,75	0
2	NAG	A	804	14/15	0.52	0.41	-	83,86,89,89	0
2	NAG	A	808	14/15	0.72	0.22	-	65,69,72,72	0
2	NAG	B	803	14/15	0.71	0.27	-	89,93,96,96	0
2	NAG	A	803	14/15	0.88	0.16	-	54,58,60,61	0
2	NAG	A	809	14/15	0.90	0.11	-	43,47,49,50	0
2	NAG	B	808	14/15	0.87	0.15	-	44,48,50,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.