wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2016 – 07:50 PM EST

PDB ID	:	1TKR
Title	:	Human Dipeptidyl Peptidase IV/CD26 inhibited with Diisopropyl FluoroPhosphate
Authors	:	Bjelke, J.R.; Christensen, J.; Branner, S.; Wagtmann, N.; Olsen, C.; Kanstrup, A.B.; Rasmussen, H.B.
Deposited on	:	2004-06-09
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

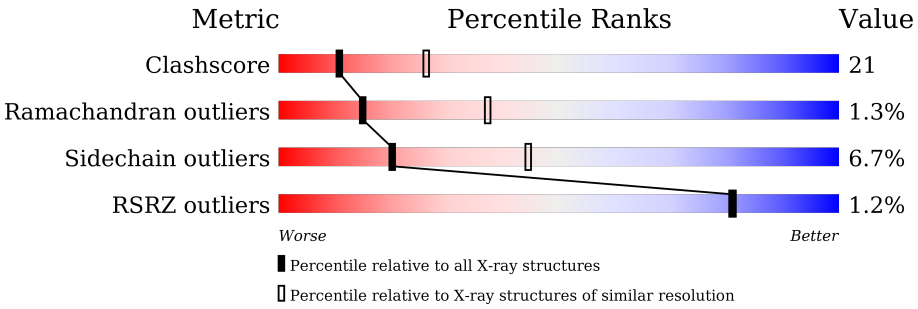
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

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

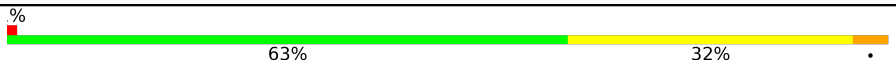
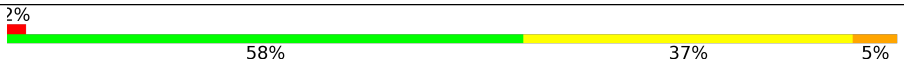
The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	
1	B	728	

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
10	NDG	B	778	-	-	X	X
10	NDG	B	779	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	DFP	A	1	-	-	-	X
4	NAG	A	774	-	-	-	X
4	NAG	A	780	-	-	-	X
5	NAG	A	775	-	-	-	X
8	NAG	B	771	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 12996 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	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			

- 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
			38	22	2	14		

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

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

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

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

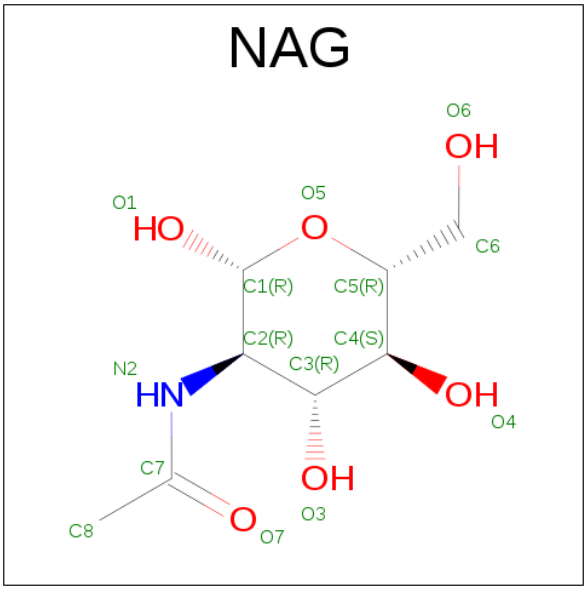
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			24	14	1	9		

- 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	B	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
			28	16	2	10		

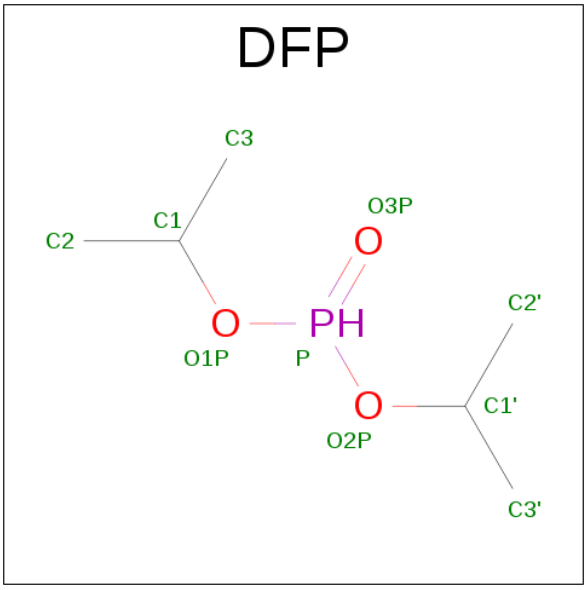
- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 11 is DIISOPROPYL PHOSPHONATE (three-letter code: DFP) (formula: $C_6H_{15}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	P	0	0
			10	6	3	1		
11	B	1	Total	C	O	P	0	0
			10	6	3	1		

- Molecule 12 is water.

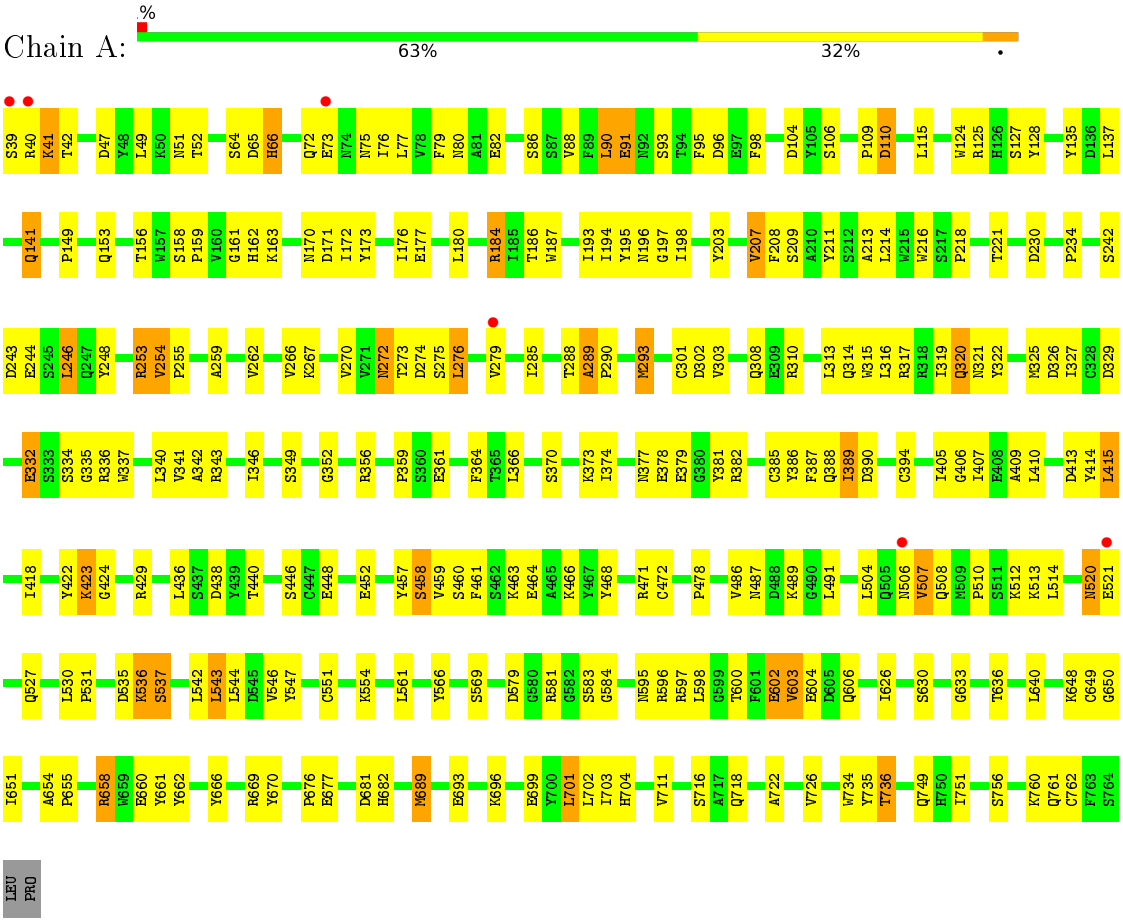
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	378	Total	O	0	0
			378	378		
12	B	315	Total	O	0	0
			315	315		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

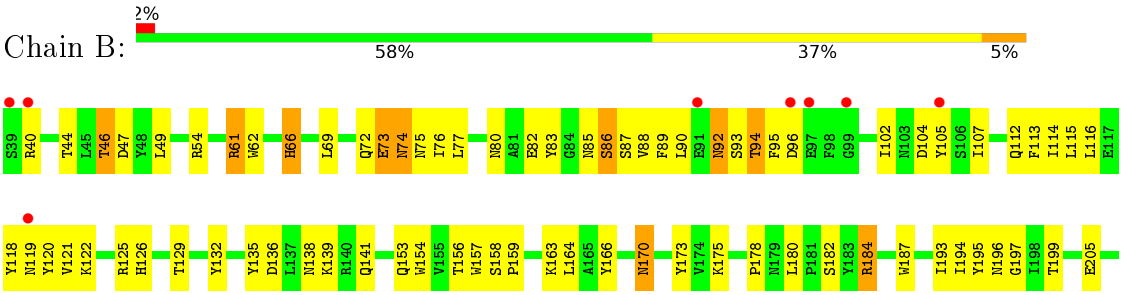
- Molecule 1: Dipeptidyl peptidase IV

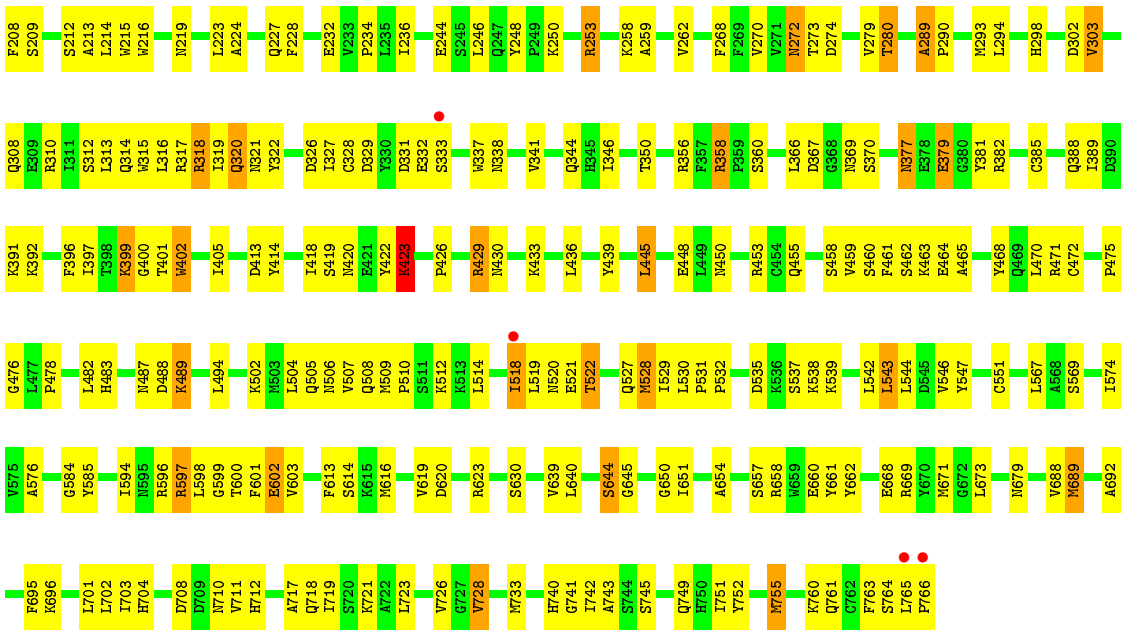
Chain A:



- Molecule 1: Dipeptidyl peptidase IV

Chain B:




F208 S209 S212 A213 L214 W215 W216 N219 L223 A224 Q227 F228 E232 V233 P234 L235 I236 E244 S245 L246 Q247 Y248 P249 K250 R253 K258 A259 V262 F268 F269 V270 V271 N272 T273 D274 V279 T280 A289 P290 M293 L294 H298 D302 V303
Q308 E309 R310 I311 S312 L313 Q314 W315 L316 R317 R318 I319 Q320 N321 Y322 D326 I327 C328 D329 Y330 D331 E332 S333 W337 N338 V341 Q344 H345 I346 T350 R356 P357 R358 F359 S360 L366 D367 G368 N369 S370 N377 E378 E379 G380 Y381 R382 C385 Q388 I389 D390
K391 K392 F396 I397 T398 K399 G400 T401 W402 I405 D413 Y414 I418 S419 N420 E421 Y422 K423 P426 R429 N430 K433 L436 Y439 L445 E448 L449 N450 R453 C454 Q455 S458 V459 S460 F461 S462 K463 E464 A465 Y468 Q469 L470 R471 C472 P475
G476 L477 P478 L482 H483 N487 D488 K489 L494 K502 K503 L504 Q505 N506 V507 Q508 M509 P510 S511 K512 K513 L514 I518 L519 N520 E521 T522 Q527 M528 I529 L530 P531 P532 D535 K536 S537 K538 K539 L542 L543 L544 D545 V546 Y547 C551 L567 A568 S569 I574
V575 A576 G584 Y585 I594 N595 R596 R597 L598 G599 T600 F601 E602 V603 F613 S614 K615 M616 V619 D620 R623 S630 V639 L640 S644 G645 G650 I651 A654 S657 R658 W659 E660 Y661 Y662 E668 R669 Y670 M671 G672 L673 N679 V688 M689 A692
F695 K696 L701 L702 I703 H704 D708 D709 N710 V711 H712 A717 Q718 I719 S720 K721 A722 L723 V726 G727 V728 M733 H740 G741 I742 A743 S744 S745 Q749 H750 I751 Y752 M755 K760 Q761 C762 F763 S764 L765 P766

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.22Å 123.46Å 131.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.60 – 2.70 30.59 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.7 (30.60-2.70) 92.4 (30.59-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.23 (at 2.68Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.203 , 0.268 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12996	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 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: BMA, NAG, DFP, NDG, FUC, 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	0.36	0/6119	0.62	0/8321
1	B	0.37	0/6136	0.61	0/8344
All	All	0.37	0/12255	0.61	0/16665

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	5948	0	5659	226	0
1	B	5964	0	5676	267	0
2	A	38	0	34	3	0
3	A	38	0	34	5	0
4	A	84	0	75	1	0
5	A	39	0	34	4	0
6	B	24	0	22	2	0
7	B	14	0	13	0	0
8	B	28	0	25	2	0
9	B	78	0	68	0	0
10	B	28	0	25	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	10	0	14	2	0
11	B	10	0	14	2	0
12	A	378	0	0	21	0
12	B	315	0	0	21	0
All	All	12996	0	11693	507	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 21.

The worst 5 of 507 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)
11:A:1:DFP:H21	12:A:1159:HOH:O	1.30	1.28
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.34	1.08
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.38	1.03
1:B:458:SER:HB3	1:B:471:ARG:HB2	1.44	0.99
1:B:358:ARG:HH11	1:B:358:ARG:HB3	1.22	0.98

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	724/728 (100%)	656 (91%)	60 (8%)	8 (1%)	17	42
1	B	726/728 (100%)	641 (88%)	74 (10%)	11 (2%)	13	32
All	All	1450/1456 (100%)	1297 (89%)	134 (9%)	19 (1%)	15	37

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	B	289	ALA
1	B	320	GLN
1	B	399	LYS
1	B	401	THR

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	651/653 (100%)	606 (93%)	45 (7%)	19	43
1	B	653/653 (100%)	610 (93%)	43 (7%)	21	45
All	All	1304/1306 (100%)	1216 (93%)	88 (7%)	20	44

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	658	ARG
1	B	74	ASN
1	B	689	MET
1	A	689	MET
1	A	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	GLN
1	B	170	ASN
1	B	712	HIS
1	B	119	ASN
1	B	138	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

27 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	$\#\|Z\|>2$
2	NAG	A	767	1,2	14,14,15	0.68	0	15,19,21	1.25	2 (13%)
2	NDG	A	768	2	14,14,15	0.67	0	15,19,21	0.88	1 (6%)
2	FUC	A	769	2	10,10,11	0.46	0	13,14,16	0.45	0
3	NDG	A	770	1,3	14,14,15	0.75	0	15,19,21	1.08	1 (6%)
3	NAG	A	771	3	14,14,15	0.67	0	15,19,21	0.72	0
3	FUC	A	772	3	10,10,11	0.50	0	13,14,16	0.34	0
4	NAG	A	773	1,4	14,14,15	0.51	0	15,19,21	0.89	0
4	NAG	A	774	4	14,14,15	0.44	0	15,19,21	0.77	1 (6%)
5	NAG	A	775	1,5	14,14,15	0.56	0	15,19,21	1.17	2 (13%)
5	NDG	A	776	5	14,14,15	0.96	1 (7%)	15,19,21	0.91	0
5	MAN	A	777	5	11,11,12	0.64	0	15,15,17	0.50	0
4	NAG	A	778	1,4	14,14,15	0.46	0	15,19,21	0.67	1 (6%)
4	NAG	A	779	4	14,14,15	0.49	0	15,19,21	0.61	0
4	NAG	A	780	1,4	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
4	NAG	A	781	4	14,14,15	0.68	0	15,19,21	0.61	0
6	NAG	B	767	1,6	14,14,15	0.51	0	15,19,21	0.71	1 (6%)
6	FUC	B	768	6	10,10,11	0.49	0	13,14,16	0.42	0
8	NDG	B	770	1,8	14,14,15	0.66	0	15,19,21	0.93	1 (6%)
8	NAG	B	771	8	14,14,15	0.48	0	15,19,21	0.83	1 (6%)
9	NAG	B	772	1,9	14,14,15	0.45	0	15,19,21	0.92	1 (6%)
9	NAG	B	773	9	14,14,15	0.45	0	15,19,21	0.83	0
9	BMA	B	774	9	11,11,12	0.59	0	15,15,17	0.22	0
9	NAG	B	775	1,9	14,14,15	0.49	0	15,19,21	0.69	0
9	NAG	B	776	9	14,14,15	0.62	0	15,19,21	1.22	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BMA	B	777	9	11,11,12	0.42	0	15,15,17	0.40	0
10	NDG	B	778	1,10	14,14,15	0.59	0	15,19,21	0.95	2 (13%)
10	NDG	B	779	10	14,14,15	0.73	1 (7%)	15,19,21	0.85	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	767	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	768	2	-	0/6/23/26	0/1/1/1
2	FUC	A	769	2	-	0/0/17/20	0/1/1/1
3	NDG	A	770	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	771	3	-	0/6/23/26	0/1/1/1
3	FUC	A	772	3	-	0/0/17/20	0/1/1/1
4	NAG	A	773	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	774	4	-	0/6/23/26	0/1/1/1
5	NAG	A	775	1,5	-	0/6/23/26	0/1/1/1
5	NDG	A	776	5	-	0/6/23/26	0/1/1/1
5	MAN	A	777	5	-	0/2/19/22	0/1/1/1
4	NAG	A	778	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	779	4	-	0/6/23/26	0/1/1/1
4	NAG	A	780	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	781	4	-	0/6/23/26	0/1/1/1
6	NAG	B	767	1,6	-	0/6/23/26	0/1/1/1
6	FUC	B	768	6	-	0/0/17/20	0/1/1/1
8	NDG	B	770	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	771	8	-	0/6/23/26	0/1/1/1
9	NAG	B	772	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	773	9	-	0/6/23/26	0/1/1/1
9	BMA	B	774	9	-	0/2/19/22	0/1/1/1
9	NAG	B	775	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	776	9	-	0/6/23/26	0/1/1/1
9	BMA	B	777	9	-	0/2/19/22	0/1/1/1
10	NDG	B	778	1,10	-	0/6/23/26	0/1/1/1
10	NDG	B	779	10	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	779	NDG	C1-C2	2.13	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	776	NDG	C1-C2	2.91	1.56	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	775	NAG	C2-N2-C7	-3.28	118.84	123.11
9	B	772	NAG	C2-N2-C7	-2.82	119.44	123.11
9	B	776	NAG	C2-N2-C7	-2.76	119.52	123.11
8	B	770	NDG	C2-N2-C7	-2.67	119.63	123.11
9	B	776	NAG	C4-C3-C2	-2.56	107.36	111.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	767	NAG	3	0
2	A	768	NDG	3	0
3	A	770	NDG	4	0
3	A	771	NAG	5	0
4	A	773	NAG	1	0
5	A	775	NAG	1	0
5	A	776	NDG	2	0
5	A	777	MAN	2	0
6	B	767	NAG	2	0
8	B	770	NDG	2	0
10	B	778	NDG	10	0
10	B	779	NDG	9	0

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	DFP	A	1	1	6,9,9	1.58	2 (33%)	6,11,11	0.41	0
11	DFP	B	1	1	6,9,9	1.60	2 (33%)	6,11,11	0.42	0
7	NAG	B	769	1	14,14,15	0.51	0	15,19,21	0.75	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	DFP	A	1	1	-	0/4/8/8	0/0/0/0
11	DFP	B	1	1	-	0/4/8/8	0/0/0/0
7	NAG	B	769	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)
11	A	1	DFP	O1P-C1	-2.69	1.42	1.46
11	B	1	DFP	O1P-C1	-2.68	1.42	1.46
11	B	1	DFP	O2P-C1'	-2.45	1.42	1.46
11	A	1	DFP	O2P-C1'	-2.33	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	769	NAG	C2-N2-C7	-2.18	120.27	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1	DFP	2	0
11	B	1	DFP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	726/728 (99%)	-0.52	6 (0%)	87 88	9, 22, 44, 67	0
1	B	728/728 (100%)	-0.36	12 (1%)	74 75	6, 24, 54, 94	0
All	All	1454/1456 (99%)	-0.44	18 (1%)	81 81	6, 23, 48, 94	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	SER	4.1
1	B	99	GLY	3.8
1	B	39	SER	3.2
1	B	97	GLU	3.1
1	A	73	GLU	3.1

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

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, 95^{th} 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
10	NDG	B	778	14/15	0.81	0.32	7.45	63,67,72,76	0
4	NAG	A	780	14/15	0.89	0.28	4.84	57,61,65,70	0
4	NAG	A	774	14/15	0.85	0.34	3.52	54,56,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	775	14/15	0.92	0.17	3.36	39,42,48,58	0
8	NAG	B	771	14/15	0.78	0.31	2.72	65,67,68,69	0
2	NAG	A	767	14/15	0.89	0.20	1.66	54,58,62,67	0
6	NAG	B	767	14/15	0.84	0.23	1.23	63,66,71,72	0
9	NAG	B	775	14/15	0.95	0.13	0.88	20,27,32,33	0
9	NAG	B	772	14/15	0.95	0.14	0.06	28,30,35,43	0
4	NAG	A	778	14/15	0.91	0.20	-	49,52,55,60	0
2	NDG	A	768	14/15	0.81	0.45	-	72,74,76,77	0
3	NAG	A	771	14/15	0.69	0.35	-	77,79,84,84	0
8	NDG	B	770	14/15	0.84	0.30	-	55,58,62,64	0
5	MAN	A	777	11/12	0.47	0.36	-	86,88,88,89	0
4	NAG	A	781	14/15	0.58	0.40	-	72,75,76,77	0
6	FUC	B	768	10/11	0.86	0.35	-	74,75,75,75	0
9	BMA	B	777	11/12	0.86	0.24	-	53,56,58,59	0
9	NAG	B	773	14/15	0.88	0.26	-	50,54,59,62	0
5	NDG	A	776	14/15	0.64	0.41	-	67,74,76,82	0
4	NAG	A	779	14/15	0.82	0.35	-	65,69,71,72	0
4	NAG	A	773	14/15	0.91	0.22	-	39,41,45,50	0
3	NDG	A	770	14/15	0.70	0.30	-	65,69,77,80	0
2	FUC	A	769	10/11	0.88	0.24	-	63,64,65,65	0
9	NAG	B	776	14/15	0.92	0.19	-	32,38,44,47	0
3	FUC	A	772	10/11	0.74	0.51	-	83,86,87,88	0
10	NDG	B	779	14/15	0.72	0.41	-	79,81,84,85	0
9	BMA	B	774	11/12	0.85	0.29	-	64,66,67,68	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(Å^2)	Q<0.9
11	DFP	A	1	10/10	0.96	0.19	3.80	16,23,27,29	0
11	DFP	B	1	10/10	0.97	0.16	0.57	25,29,35,35	0
7	NAG	B	769	14/15	0.77	0.39	-	68,73,74,75	0

6.5 Other polymers (i)

There are no such residues in this entry.