wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:23 AM GMT

PDB ID	:	2QJR
Title	:	dipepdyl peptidase IV in complex with inhibitor PZF
Authors	:	Shenping, L.
Deposited on	:	2007-07-09
Resolution	:	2.20 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:

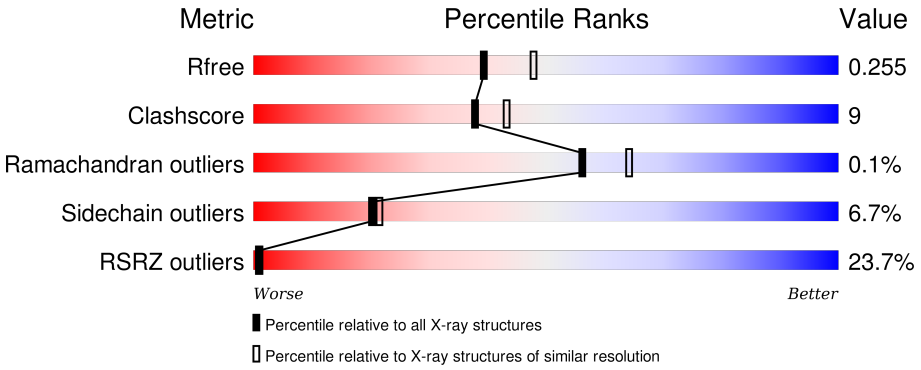
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	748	26% 75% 20%
1	B	748	20% 69% 23% 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	800	-	-	-	X
3	LGU	A	802	X	-	-	-
3	LGU	A	804	X	-	-	-
4	NAG	B	796	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12532 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	C	N	O	S	0	0	0
			5957	3825	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	LEU	-	EXPRESSION TAG	UNP P27487
A	768	VAL	-	EXPRESSION TAG	UNP P27487
A	769	PRO	-	EXPRESSION TAG	UNP P27487
A	770	ARG	-	EXPRESSION TAG	UNP P27487
A	771	GLY	-	EXPRESSION TAG	UNP P27487
A	772	SER	-	EXPRESSION TAG	UNP P27487
A	773	HIS	-	EXPRESSION TAG	UNP P27487
A	774	HIS	-	EXPRESSION TAG	UNP P27487
A	775	HIS	-	EXPRESSION TAG	UNP P27487
A	776	HIS	-	EXPRESSION TAG	UNP P27487
A	777	HIS	-	EXPRESSION TAG	UNP P27487
A	778	HIS	-	EXPRESSION TAG	UNP P27487
B	767	LEU	-	EXPRESSION TAG	UNP P27487
B	768	VAL	-	EXPRESSION TAG	UNP P27487
B	769	PRO	-	EXPRESSION TAG	UNP P27487
B	770	ARG	-	EXPRESSION TAG	UNP P27487
B	771	GLY	-	EXPRESSION TAG	UNP P27487
B	772	SER	-	EXPRESSION TAG	UNP P27487
B	773	HIS	-	EXPRESSION TAG	UNP P27487
B	774	HIS	-	EXPRESSION TAG	UNP P27487
B	775	HIS	-	EXPRESSION TAG	UNP P27487
B	776	HIS	-	EXPRESSION TAG	UNP P27487
B	777	HIS	-	EXPRESSION TAG	UNP P27487
B	778	HIS	-	EXPRESSION TAG	UNP P27487

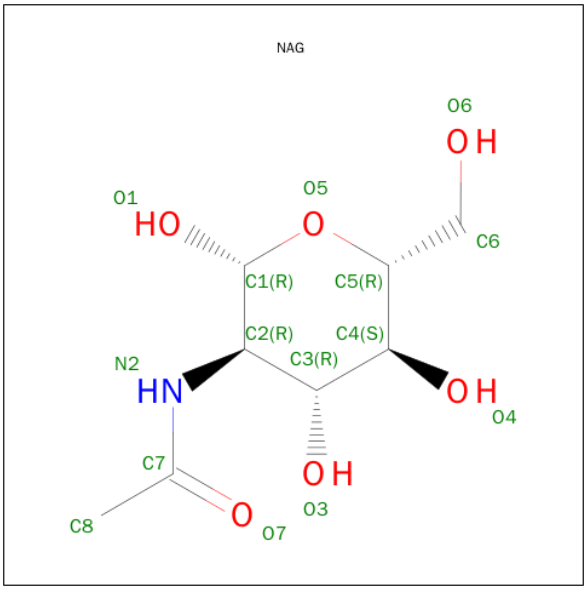
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total C N O 61 34 2 25	0	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

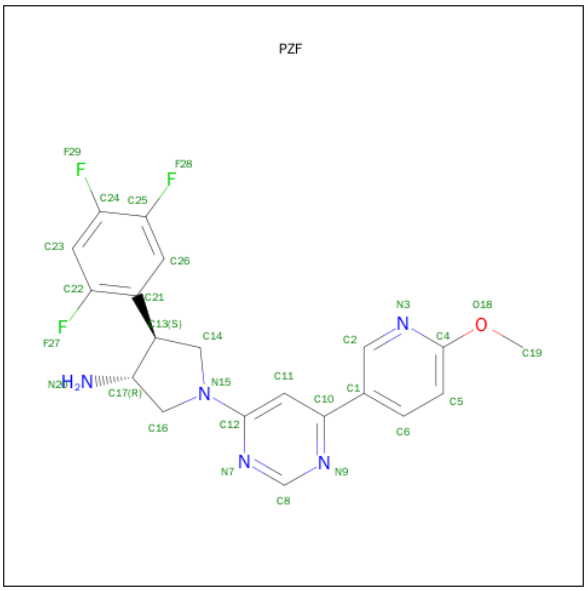


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

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

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

- Molecule 6 is (3R,4S)-1-[6-(6-METHOXYPYRIDIN-3-YL)PYRIMIDIN-4-YL]-4-(2,4,5-TRIFLUOROPHENYL)PYRROLIDIN-3-AMINE (three-letter code: PZF) (formula: $C_{20}H_{18}F_3N_5O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C F N O 29 20 3 5 1	0	0
6	B	1	Total C F N O 29 20 3 5 1	0	0

- Molecule 7 is water.

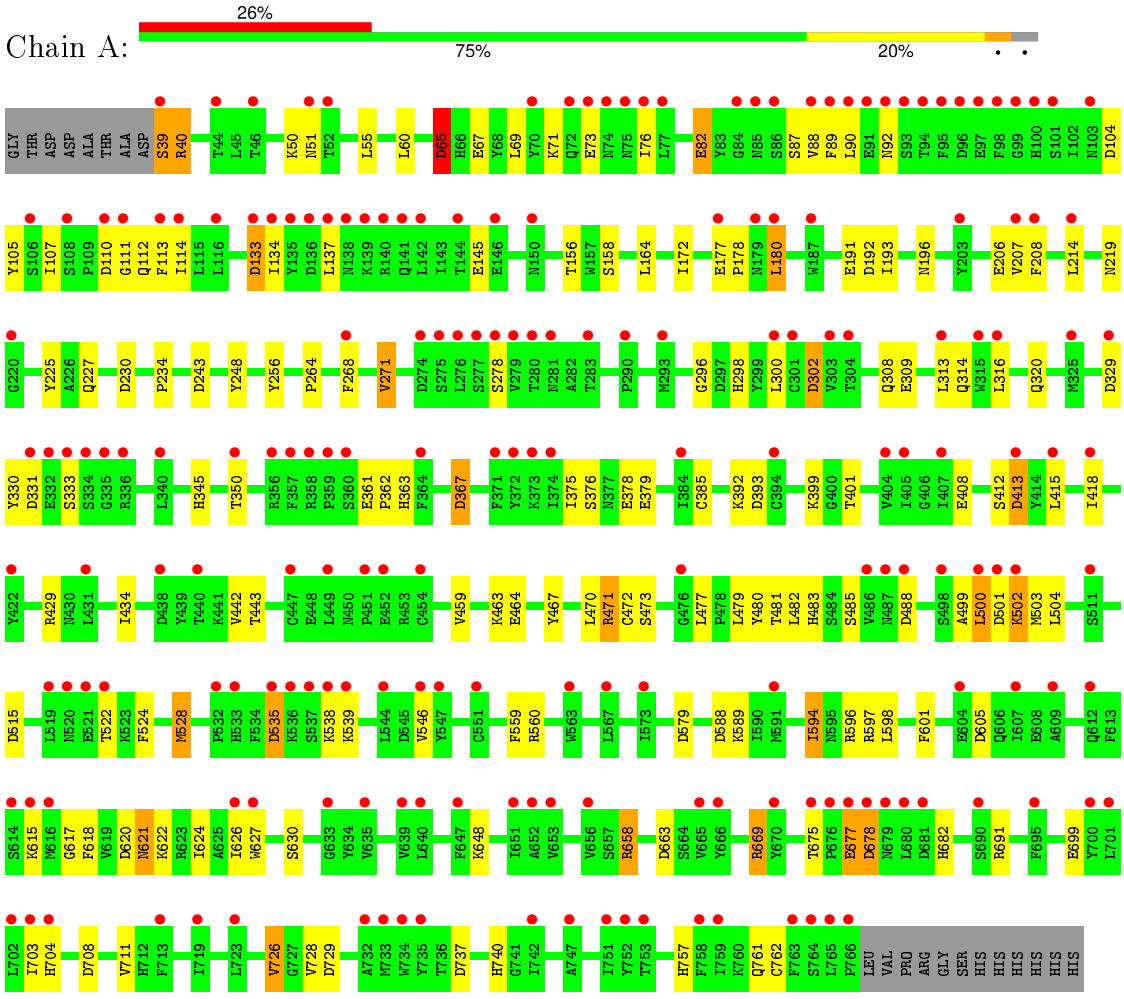
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	105	Total O 105 105	0	0
7	B	226	Total O 226 226	0	0

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.

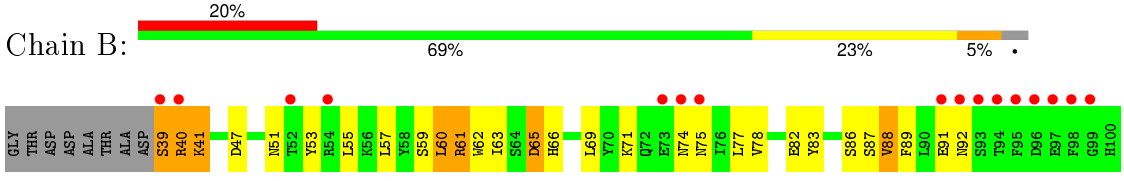
- Molecule 1: Dipeptidyl peptidase 4

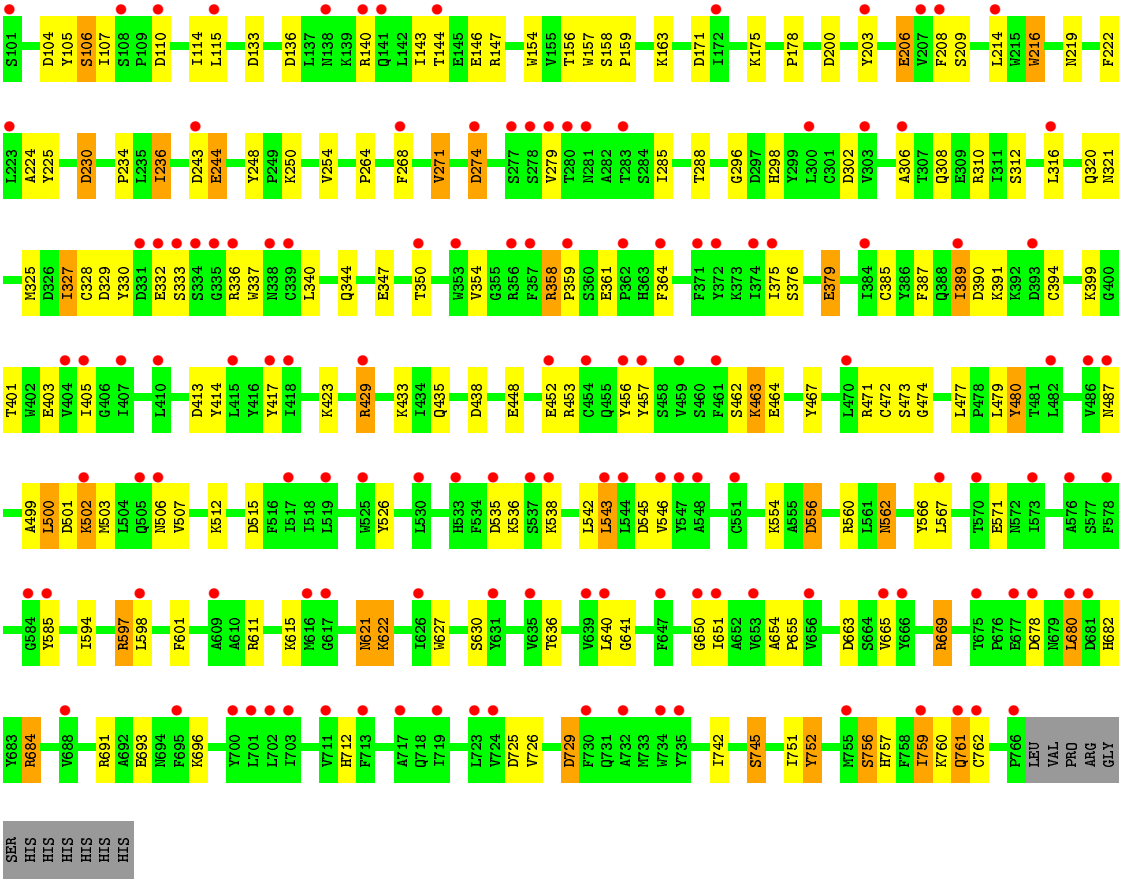
Chain A:



- Molecule 1: Dipeptidyl peptidase 4

Chain B:




S101 D104 Y105 S106 I107 S108 P109 D110 I114 L115 D133 D136 L137 N138 K139 R140 Q141 L142 I143 T144 E145 E146 R147 W454 Y155 T156 W457 S158 P159 K163 D171 I172 K175 P178 D200 Y203 E206 Y207 F208 S209 L214 W215 W216 N219 F222
L223 A224 Y225 D230 P234 L235 I236 D243 E244 Y248 P249 K250 V254 P264 F268 V271 D274 S277 S278 V279 T280 N281 A282 T283 S284 I285 T288 G296 D297 H298 Y299 L300 C301 D302 V303 A306 T307 Q308 E309 R310 I311 S312 L316 Q320 N321
M325 D326 I327 C328 D329 Y330 D331 E332 S333 S334 G335 R336 W337 N338 C339 L340 Q344 E347 T350 W353 V354 G355 R356 F357 R358 P359 S360 E361 P362 H363 F364 F371 Y372 K373 I374 I375 S376 E379 I384 C385 Y386 F387 Q388 I389 D390 K391 K392 D393 C394 K399 G400
T401 W402 E403 Y404 I405 G406 I407 L410 D413 Y414 L415 Y416 Y417 I418 K423 R429 K433 I434 Q435 D438 E448 E452 R453 C454 Q455 Y456 Y457 S458 Y459 S460 F461 S462 K463 E464 Y467 L470 R471 C472 S473 G474 L477 P478 L479 Y480 T481 L482 V486 N487
A499 L500 D501 K502 M503 L504 Q505 N506 V507 K512 D515 F516 I517 I518 L519 W525 Y526 L530 H533 F534 D535 K536 S537 K538 L542 L543 L544 D545 V546 Y547 A548 C551 K554 A555 D556 R560 L561 N562 Y566 L567 T570 E571 N572 I573 A576 S577 F578
G584 Y585 I594 R597 L598 F601 A609 A610 R611 K615 M616 G617 N621 K622 I626 W627 S630 Y631 V635 T636 V639 L640 G641 F647 G650 I651 A652 V653 A654 P655 V656 D663 S664 V665 Y666 R669 T675 P676 E677 D678 N679 L680 D681 H682
Y683 R684 V688 R691 A692 P693 N694 F695 K696 Y700 L701 L702 I703 V711 H712 F713 A717 Q718 I719 L723 V724 D725 V726 D729 F730 Q731 A732 M733 W734 Y735 I742 S745 I751 Y752 M755 S756 H757 F758 I759 K760 Q761 C762 P766 LEU VAL PRO ARG GLY
SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.47Å 68.80Å 422.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.90 – 2.20 41.90 – 2.19	Depositor EDS
% Data completeness (in resolution range)	85.7 (41.90-2.20) 85.4 (41.90-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.191 , 0.253 0.200 , 0.255	Depositor DCC
R_{free} test set	4236 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.929	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.7	EDS
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	2 of 85287 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12532	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MAN, PZF, NAG, NDG, LGU

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	1.12	6/6129 (0.1%)	1.09	33/8336 (0.4%)
1	B	1.43	42/6129 (0.7%)	1.24	43/8336 (0.5%)
All	All	1.29	48/12258 (0.4%)	1.17	76/16672 (0.5%)

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
3	A	2	0

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	385	CYS	CB-SG	-8.03	1.68	1.82
1	B	250	LYS	CD-CE	6.76	1.68	1.51
1	B	244	GLU	CD-OE1	6.63	1.32	1.25
1	B	83	TYR	CE1-CZ	6.46	1.47	1.38
1	B	82	GLU	CD-OE1	6.43	1.32	1.25

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	669	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	A	669	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	B	453	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	B	61	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	658	ARG	NE-CZ-NH1	10.27	125.44	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	802	LGU	C5
3	A	804	LGU	C5

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5957	0	5672	94	0
1	B	5957	0	5672	125	0
2	A	56	0	50	1	0
2	B	28	0	25	1	0
3	A	61	0	48	0	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
5	B	56	0	50	2	0
6	A	29	0	18	1	0
6	B	29	0	18	0	0
7	A	105	0	0	10	0
7	B	226	0	0	21	0
All	All	12532	0	11579	218	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 9.

The worst 5 of 218 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:39:SER:O	1:A:40:ARG:CZ	1.79	1.29
1:B:40:ARG:HD3	1:B:40:ARG:N	1.64	1.12
1:B:39:SER:HB2	1:B:40:ARG:HD2	1.31	1.08
1:B:597:ARG:HD3	7:B:1038:HOH:O	1.56	1.02
1:A:621:ASN:C	1:A:621:ASN:HD22	1.64	0.99

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	726/748 (97%)	694 (96%)	31 (4%)	1 (0%)	56	64
1	B	726/748 (97%)	689 (95%)	36 (5%)	1 (0%)	56	64
All	All	1452/1496 (97%)	1383 (95%)	67 (5%)	2 (0%)	56	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	630	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	651/669 (97%)	610 (94%)	41 (6%)	22	24
1	B	651/669 (97%)	605 (93%)	46 (7%)	18	19
All	All	1302/1338 (97%)	1215 (93%)	87 (7%)	20	21

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	726	VAL

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Mol	Chain	Res	Type
1	B	88	VAL
1	B	621	ASN
1	A	762	CYS
1	B	51	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	748	HIS
1	B	123	GLN
1	B	682	HIS
1	A	757	HIS
1	A	263	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)

15 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	794	1,2	14,14,15	1.46	3 (21%)	15,19,21	1.61	2 (13%)
3	NAG	A	796	1,3	14,14,15	1.25	2 (14%)	15,19,21	2.04	7 (46%)
2	NAG	A	797	2	14,14,15	0.84	0	15,19,21	2.15	7 (46%)
3	NAG	A	798	3	14,14,15	0.88	0	15,19,21	1.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	800	1,2	14,14,15	0.69	0	15,19,21	2.32	4 (26%)
2	NAG	A	801	2	14,14,15	0.80	1 (7%)	15,19,21	1.30	1 (6%)
3	LGU	A	802	3	11,11,13	0.82	1 (9%)	14,15,19	2.52	5 (35%)
3	MAN	A	803	3	11,11,12	1.04	1 (9%)	14,15,17	1.72	1 (7%)
3	LGU	A	804	3	11,11,13	0.87	0	14,15,19	2.02	4 (28%)
2	NAG	B	794	1,2	14,14,15	1.16	1 (7%)	15,19,21	1.48	3 (20%)
2	NAG	B	797	2	14,14,15	1.16	1 (7%)	15,19,21	1.78	5 (33%)
5	NDG	B	799	1,5	14,14,15	1.11	1 (7%)	15,19,21	1.50	3 (20%)
5	NDG	B	800	1,5	14,14,15	0.85	1 (7%)	15,19,21	1.31	2 (13%)
5	NAG	B	801	5	14,14,15	0.63	0	15,19,21	1.66	3 (20%)
5	NAG	B	805	5	14,14,15	0.52	0	15,19,21	1.60	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	794	1,2	-	0/6/23/26	0/1/1/1
3	NAG	A	796	1,3	-	0/6/23/26	0/1/1/1
2	NAG	A	797	2	-	0/6/23/26	0/1/1/1
3	NAG	A	798	3	-	0/6/23/26	0/1/1/1
2	NAG	A	800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	801	2	-	0/6/23/26	0/1/1/1
3	LGU	A	802	3	1/1/4/6	0/2/19/24	0/1/1/1
3	MAN	A	803	3	-	0/2/19/22	0/1/1/1
3	LGU	A	804	3	1/1/4/6	0/2/19/24	0/1/1/1
2	NAG	B	794	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	797	2	-	0/6/23/26	0/1/1/1
5	NDG	B	799	1,5	-	0/6/23/26	0/1/1/1
5	NDG	B	800	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	801	5	-	0/6/23/26	0/1/1/1
5	NAG	B	805	5	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	797	NAG	O5-C1	-3.44	1.38	1.43
3	A	796	NAG	O5-C1	-3.39	1.38	1.43
2	A	794	NAG	C2-N2	-3.06	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	794	NAG	O5-C1	-3.05	1.38	1.43
5	B	800	NDG	O-C1	-2.62	1.39	1.43

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	MAN	O5-C1-C2	-5.50	101.93	110.86
3	A	802	LGU	C1-C2-C3	-4.85	103.80	109.54
3	A	804	LGU	O5-C1-C2	-4.36	103.78	110.86
3	A	804	LGU	C1-O5-C5	-3.95	107.24	112.25
3	A	796	NAG	O3-C3-C4	-3.16	103.22	110.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	802	LGU	C5
3	A	804	LGU	C5

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	794	NAG	1	0
2	A	797	NAG	1	0
2	B	794	NAG	1	0
5	B	800	NDG	1	0
5	B	805	NAG	1	0

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	799	1	14,14,15	0.88	0	15,19,21	1.44	2 (13%)
6	PZF	A	900	-	32,32,32	1.03	2 (6%)	41,46,46	2.29	13 (31%)
4	NAG	B	796	1	14,14,15	1.10	1 (7%)	15,19,21	2.37	6 (40%)
6	PZF	B	900	-	32,32,32	1.57	8 (25%)	41,46,46	2.64	15 (36%)

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	799	1	-	0/6/23/26	0/1/1/1
6	PZF	A	900	-	-	0/14/26/26	0/4/4/4
4	NAG	B	796	1	-	0/6/23/26	0/1/1/1
6	PZF	B	900	-	-	0/14/26/26	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	796	NAG	O5-C1	-3.44	1.38	1.43
6	B	900	PZF	C26-C21	-3.18	1.34	1.39
6	B	900	PZF	C21-C13	-3.16	1.47	1.52
6	B	900	PZF	F29-C24	-2.93	1.28	1.35
6	A	900	PZF	C21-C13	-2.78	1.48	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	900	PZF	N7-C8-N9	-5.00	120.25	128.67
4	B	796	NAG	O4-C4-C5	-4.77	96.60	109.24
6	B	900	PZF	N7-C8-N9	-4.20	121.59	128.67
6	A	900	PZF	C11-C10-N9	-3.73	117.11	122.02
6	B	900	PZF	C11-C12-N7	-3.30	116.60	122.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	900	PZF	1	0
4	B	796	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	728/748 (97%)	1.58	196 (26%)	1	1	46, 55, 70, 79	0
1	B	728/748 (97%)	1.38	149 (20%)	1	1	44, 55, 71, 79	0
All	All	1456/1496 (97%)	1.48	345 (23%)	1	1	44, 55, 71, 79	0

The worst 5 of 345 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	SER	9.8
1	A	279	VAL	8.9
1	A	74	ASN	8.5
1	A	93	SER	8.0
1	A	94	THR	7.9

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
2	NAG	A	800	14/15	0.73	0.33	4.72	81,87,90,94	0
3	NAG	A	796	14/15	0.85	0.25	1.89	51,59,64,69	0
5	NDG	B	800	14/15	0.86	0.30	1.71	75,84,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	B	805	14/15	0.80	0.33	1.45	87,91,94,95	0
2	NAG	A	794	14/15	0.92	0.24	0.51	44,48,53,63	0
2	NAG	B	794	14/15	0.92	0.13	-2.22	42,47,56,61	0
2	NAG	A	797	14/15	0.76	0.30	-	75,83,85,86	0
2	NAG	B	797	14/15	0.84	0.28	-	63,68,78,80	0
5	NAG	B	801	14/15	0.69	0.48	-	96,100,102,103	0
3	NAG	A	798	14/15	0.69	0.42	-	65,76,79,83	0
2	NAG	A	801	14/15	0.75	0.52	-	99,102,104,105	0
5	NDG	B	799	14/15	0.84	0.39	-	79,85,92,93	0
3	LGU	A	804	11/13	0.55	0.44	-	87,93,96,98	0
3	MAN	A	803	11/12	0.83	0.40	-	89,91,93,96	0
3	LGU	A	802	11/13	0.83	0.49	-	88,93,97,98	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
4	NAG	B	796	14/15	0.89	0.24	2.16	54,59,68,72	0
6	PZF	A	900	29/29	0.95	0.14	-2.65	44,57,71,80	0
6	PZF	B	900	29/29	0.97	0.12	-3.13	35,44,62,72	0
4	NAG	A	799	14/15	0.78	0.34	-	77,82,87,88	0

6.5 Other polymers

There are no such residues in this entry.