



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:56 PM GMT

PDB ID : 3VJM  
Title : Crystal structure of human deipeptidyl peptidase IV (DPP-4) in complex with a prolylthiazolidine inhibitor #1  
Authors : Akahoshi, F.; Kishida, H.; Miyaguchi, I.; Yoshida, T.; Ishii, S.  
Deposited on : 2011-10-24  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

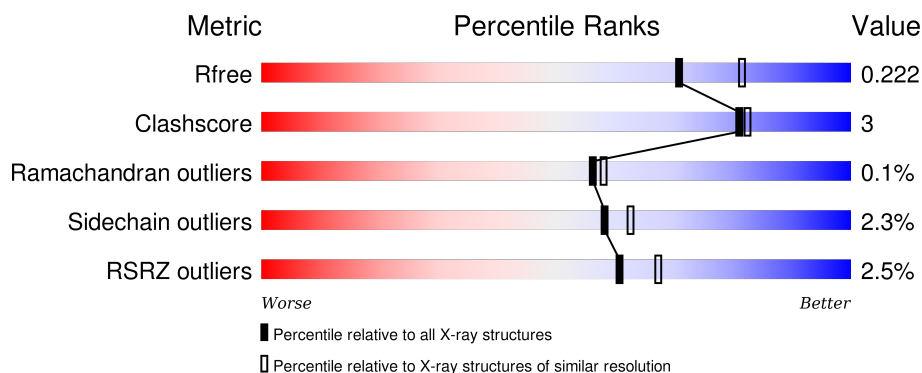
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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	740	<div> <div>3%</div> <div>90%</div> <div>8% ..</div> </div>
1	B	740	<div> <div>2%</div> <div>90%</div> <div>7% ..</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
3	NAG	A	1321	-	-	-	X
4	NAG	A	1219	-	-	-	X
4	NAG	A	1220	-	-	-	X
4	NAG	B	1219	-	-	-	X
4	NAG	B	1220	-	-	-	X
4	NAG	B	1321	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13231 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.

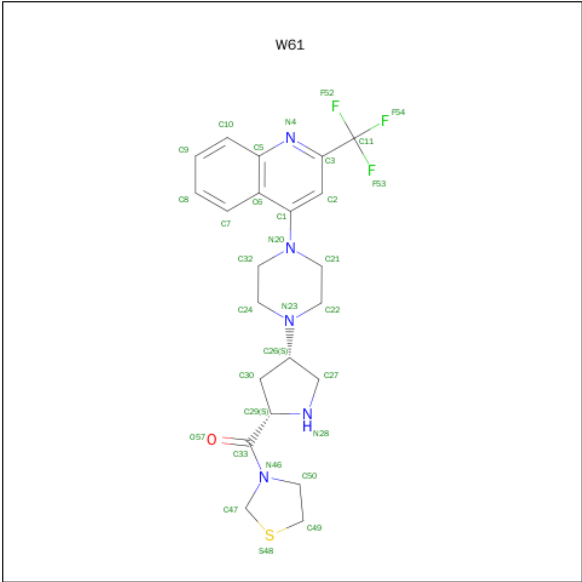
- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5971	3831	983	1131	26			
1	B	729	Total	C	N	O	S	0	0	0
			5971	3831	983	1131	26			

There are 12 discrepancies between the modelled and reference sequences:

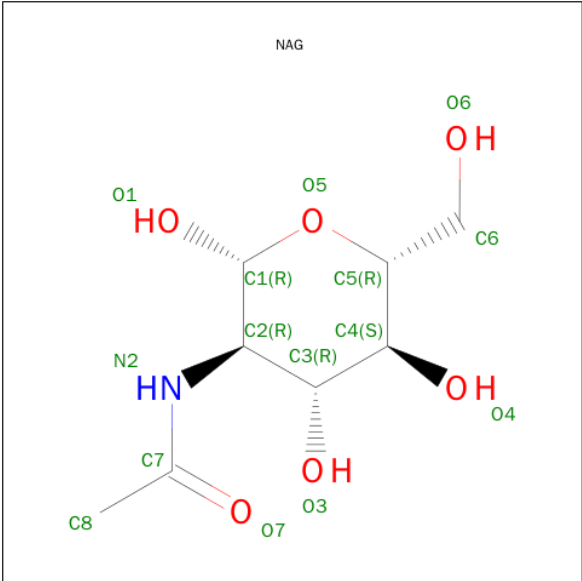
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	HIS	-	EXPRESSION TAG	UNP P27487
A	768	HIS	-	EXPRESSION TAG	UNP P27487
A	769	HIS	-	EXPRESSION TAG	UNP P27487
A	770	HIS	-	EXPRESSION TAG	UNP P27487
A	771	HIS	-	EXPRESSION TAG	UNP P27487
A	772	HIS	-	EXPRESSION TAG	UNP P27487
B	767	HIS	-	EXPRESSION TAG	UNP P27487
B	768	HIS	-	EXPRESSION TAG	UNP P27487
B	769	HIS	-	EXPRESSION TAG	UNP P27487
B	770	HIS	-	EXPRESSION TAG	UNP P27487
B	771	HIS	-	EXPRESSION TAG	UNP P27487
B	772	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is 1,3-THIAZOLIDIN-3-YL[(2S,4S)-4-{4-[2-(TRIFLUOROMETHYL)QUINOLIN-4-YL]PIPERAZIN-1-YL}PYRROLIDIN-2-YL]METHANONE (three-letter code: W61) (formula: C<sub>22</sub>H<sub>26</sub>F<sub>3</sub>N<sub>5</sub>OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			32	22	3	5	1	1		
2	B	1	Total	C	F	N	O	S	0	0
			32	22	3	5	1	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- 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	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

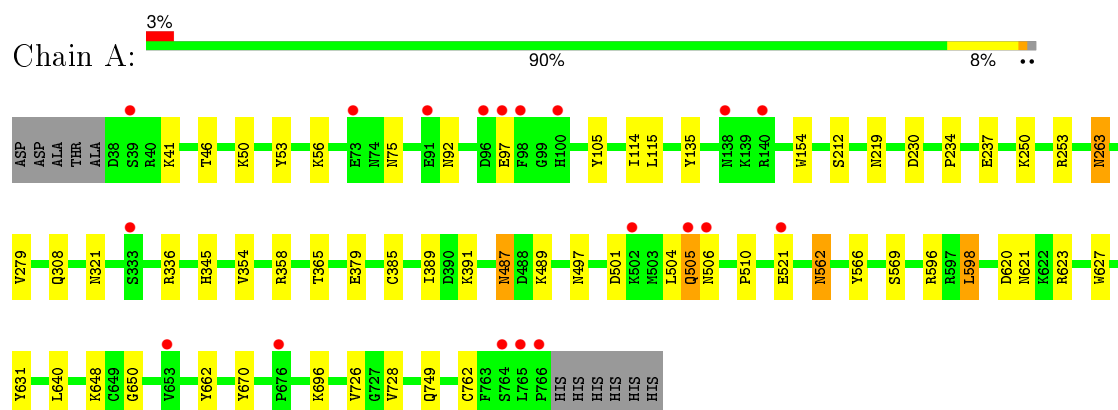
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	478	Total	O	0	0
			478	478		
5	B	509	Total	O	0	0
			509	509		

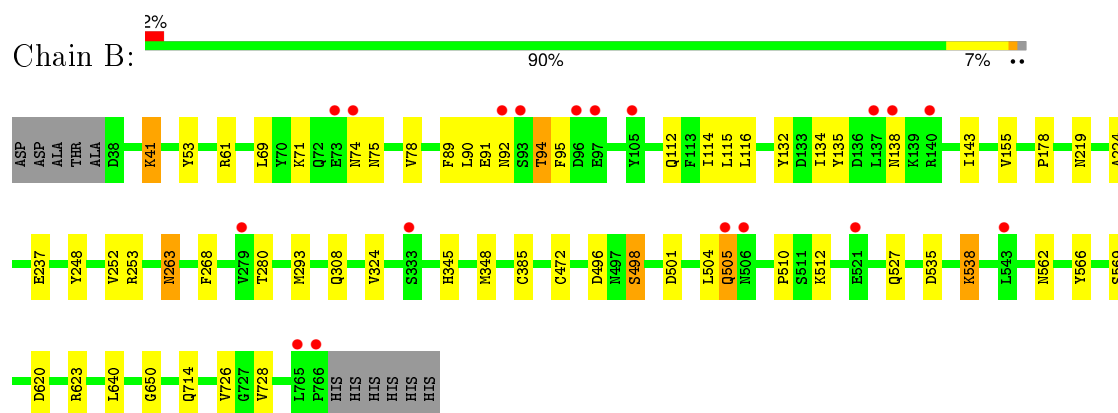
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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



#### • Molecule 1: Dipeptidyl peptidase 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.95Å 125.94Å 137.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 31.35 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.00-2.10) 91.8 (31.35-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.185 , 0.224 0.186 , 0.222	Depositor DCC
$R_{free}$ test set	5446 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 109648 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W61, 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	0.53	0/6143	0.61	0/8355
1	B	0.54	0/6143	0.62	0/8355
All	All	0.53	0/12286	0.61	0/16710

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	5971	0	5683	38	0
1	B	5971	0	5683	37	0
2	A	32	0	26	3	0
2	B	32	0	26	1	0
3	A	56	0	52	2	0
3	B	42	0	39	0	0
4	A	56	0	50	1	0
4	B	84	0	75	0	0
5	A	478	0	0	7	0
5	B	509	0	0	3	0
All	All	13231	0	11634	78	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 3.

All (78) 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)
3:A:1229:NAG:H81	5:A:2141:HOH:O	1.75	0.86
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.26	0.83
1:B:69:LEU:HD23	1:B:78:VAL:HG22	1.65	0.79
1:B:91:GLU:O	1:B:94:THR:HG22	1.86	0.75
1:B:219:ASN:H	1:B:308:GLN:HE22	1.35	0.74
1:B:345:HIS:HD2	5:B:2693:HOH:O	1.77	0.68
1:A:219:ASN:H	1:A:308:GLN:HE22	1.43	0.67
1:A:620:ASP:OD2	1:A:623:ARG:HD3	1.95	0.66
1:B:75:ASN:ND2	1:B:92:ASN:H	1.94	0.64
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.80	0.63
1:B:41:LYS:HE3	1:B:53:TYR:OH	1.99	0.63
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.80	0.61
1:B:41:LYS:HG2	5:B:2776:HOH:O	2.02	0.59
1:A:391:LYS:HE3	5:A:2291:HOH:O	2.05	0.56
1:B:293:MET:HE3	1:B:324:VAL:HG12	1.87	0.56
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.87	0.55
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.88	0.55
1:B:496:ASP:OD1	1:B:498:SER:HB2	2.06	0.55
1:B:620:ASP:OD1	1:B:623:ARG:HD3	2.08	0.54
1:A:505:GLN:HA	1:A:505:GLN:HE21	1.72	0.54
1:B:501:ASP:O	1:B:505:GLN:HG2	2.09	0.53
1:B:293:MET:CE	1:B:324:VAL:HG12	2.39	0.53
1:A:279:VAL:HG22	5:A:2258:HOH:O	2.09	0.52
1:B:71:LYS:HD3	1:B:74:ASN:HA	1.91	0.51
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.93	0.50
1:B:535:ASP:HB3	1:B:538:LYS:HG3	1.92	0.50
1:B:90:LEU:HD21	1:B:95:PHE:HE1	1.77	0.50
1:A:50:LYS:HE3	1:A:749:GLN:OE1	2.12	0.49
1:A:501:ASP:O	1:A:505:GLN:HG2	2.13	0.49
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.40	0.48
1:A:621:ASN:HD22	1:A:621:ASN:H	1.61	0.47
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.97	0.47
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.50	0.47
4:A:1219:NAG:H82	5:A:2262:HOH:O	2.15	0.47
1:B:219:ASN:N	1:B:308:GLN:HE22	2.08	0.46
1:A:46:THR:HG23	5:A:2260:HOH:O	2.14	0.46
1:A:41:LYS:HE2	1:A:53:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:ND2	1:A:92:ASN:H	2.14	0.45
1:B:112:GLN:HG2	1:B:138:ASN:HD21	1.82	0.45
1:A:345:HIS:HE1	1:A:389:ILE:O	1.99	0.45
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.16	0.45
1:A:365:THR:HG22	5:A:2192:HOH:O	2.17	0.45
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.98	0.44
3:A:1092:NAG:H3	3:A:1092:NAG:H83	2.00	0.44
1:B:143:ILE:HD12	1:B:178:PRO:HB2	2.00	0.43
1:A:648:LYS:HD3	1:A:762:CYS:SG	2.59	0.43
1:B:237:GLU:HA	1:B:252:VAL:O	2.17	0.43
1:A:640:LEU:HD11	1:A:650:GLY:HA3	2.00	0.43
2:A:1000:W61:H29	2:A:1000:W61:H50A	1.90	0.43
1:B:726:VAL:HG23	1:B:728:VAL:HG23	2.00	0.43
1:B:115:LEU:HD21	1:B:155:VAL:HG11	2.00	0.43
1:B:640:LEU:HD11	1:B:650:GLY:HA3	2.01	0.43
1:A:596:ARG:N	1:A:670:TYR:O	2.51	0.42
1:A:562:ASN:C	1:A:562:ASN:HD22	2.22	0.42
1:A:621:ASN:ND2	1:A:621:ASN:H	2.17	0.42
1:B:512:LYS:HD3	5:B:2598:HOH:O	2.19	0.42
1:B:134:ILE:HD13	1:B:178:PRO:HB3	2.02	0.42
1:A:358:ARG:NH1	2:A:1000:W61:H8	2.35	0.42
1:A:321:ASN:HA	1:A:354:VAL:HG23	2.01	0.42
1:A:263:ASN:HA	1:A:263:ASN:HD22	1.66	0.41
1:A:598:LEU:HG	1:A:631:TYR:OH	2.20	0.41
1:B:75:ASN:HD22	1:B:91:GLU:HA	1.86	0.41
1:A:662:TYR:OH	2:A:1000:W61:C33	2.68	0.41
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.01	0.41
2:B:1000:W61:H50A	2:B:1000:W61:H29	1.89	0.41
1:B:505:GLN:HE21	1:B:505:GLN:HA	1.85	0.41
1:A:105:TYR:HA	1:A:115:LEU:O	2.20	0.41
1:B:263:ASN:HA	1:B:263:ASN:HD22	1.66	0.41
1:B:116:LEU:O	1:B:132:TYR:HA	2.20	0.41
1:B:143:ILE:CD1	1:B:178:PRO:HB2	2.51	0.41
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.56	0.41
1:A:219:ASN:N	1:A:308:GLN:HE22	2.14	0.41
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.50	0.41
1:A:345:HIS:HD2	5:A:2081:HOH:O	2.03	0.41
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.56	0.41
1:B:512:LYS:HE3	1:B:527:GLN:CD	2.41	0.40
1:A:510:PRO:HD3	1:A:569:SER:HB2	2.03	0.40
1:A:487:ASN:CG	1:A:489:LYS:HG2	2.41	0.40

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	727/740 (98%)	699 (96%)	28 (4%)	0	100	100
1	B	727/740 (98%)	704 (97%)	22 (3%)	1 (0%)	56	58
All	All	1454/1480 (98%)	1403 (96%)	50 (3%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	714	GLN

### 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	654/663 (99%)	638 (98%)	16 (2%)	57	61
1	B	654/663 (99%)	640 (98%)	14 (2%)	61	66
All	All	1308/1326 (99%)	1278 (98%)	30 (2%)	58	62

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	230	ASP

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Mol	Chain	Res	Type
1	A	250	LYS
1	A	263	ASN
1	A	336	ARG
1	A	379	GLU
1	A	385	CYS
1	A	487	ASN
1	A	504	LEU
1	A	505	GLN
1	A	506	ASN
1	A	521	GLU
1	A	562	ASN
1	A	566	TYR
1	A	598	LEU
1	A	627	TRP
1	B	41	LYS
1	B	61	ARG
1	B	94	THR
1	B	263	ASN
1	B	280	THR
1	B	348	MET
1	B	385	CYS
1	B	472	CYS
1	B	498	SER
1	B	504	LEU
1	B	505	GLN
1	B	538	LYS
1	B	562	ASN
1	B	566	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	112	GLN
1	A	141	GLN
1	A	169	ASN
1	A	263	ASN
1	A	286	GLN
1	A	308	GLN
1	A	345	HIS
1	A	487	ASN
1	A	505	GLN

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Mol	Chain	Res	Type
1	A	506	ASN
1	A	562	ASN
1	A	572	ASN
1	A	621	ASN
1	A	679	ASN
1	A	694	ASN
1	A	697	GLN
1	B	75	ASN
1	B	138	ASN
1	B	169	ASN
1	B	263	ASN
1	B	286	GLN
1	B	308	GLN
1	B	345	HIS
1	B	505	GLN
1	B	562	ASN
1	B	572	ASN
1	B	679	ASN
1	B	694	ASN

### 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 ⓘ

10 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1219	1,4	14,14,15	0.56	0	15,19,21	0.87	0
4	NAG	A	1220	4	14,14,15	0.59	0	15,19,21	1.50	3 (20%)
4	NAG	A	1281	1,4	14,14,15	0.70	0	15,19,21	0.83	0
4	NAG	A	1282	4	14,14,15	0.49	0	15,19,21	1.09	1 (6%)
4	NAG	B	1219	1,4	14,14,15	0.47	0	15,19,21	0.82	0
4	NAG	B	1220	4	14,14,15	0.49	0	15,19,21	1.09	1 (6%)
4	NAG	B	1229	1,4	14,14,15	0.59	0	15,19,21	1.24	1 (6%)
4	NAG	B	1230	4	14,14,15	0.50	0	15,19,21	1.11	1 (6%)
4	NAG	B	1321	1,4	14,14,15	0.52	0	15,19,21	0.86	1 (6%)
4	NAG	B	1322	4	14,14,15	0.49	0	15,19,21	2.06	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1219	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1220	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1281	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1282	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1219	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1220	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1229	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1230	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1321	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1322	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1220	NAG	C3-C4-C5	-2.24	106.29	110.20
4	B	1322	NAG	C4-C3-C2	2.28	114.78	111.23
4	B	1321	NAG	C1-O5-C5	2.29	115.15	112.25
4	A	1220	NAG	C4-C3-C2	2.34	114.87	111.23
4	B	1230	NAG	C1-O5-C5	2.39	115.28	112.25
4	A	1220	NAG	C3-C4-C5	3.13	115.65	110.20
4	A	1282	NAG	C1-O5-C5	3.19	116.30	112.25
4	A	1220	NAG	C1-O5-C5	3.23	116.35	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1322	NAG	C3-C4-C5	3.39	116.11	110.20
4	B	1229	NAG	C1-O5-C5	4.01	117.34	112.25
4	B	1322	NAG	C1-O5-C5	6.32	120.26	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1219	NAG	1	0

## 5.6 Ligand geometry

9 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	$\# Z  > 2$
2	W61	A	1000	-	34,36,36	1.05	1 (2%)	46,53,53	2.21	11 (23%)
3	NAG	A	1085	1	14,14,15	0.39	0	15,19,21	2.18	1 (6%)
3	NAG	A	1092	1	14,14,15	0.52	0	15,19,21	2.40	6 (40%)
3	NAG	A	1229	1	14,14,15	0.46	0	15,19,21	1.31	1 (6%)
3	NAG	A	1321	1	14,14,15	0.48	0	15,19,21	1.94	2 (13%)
2	W61	B	1000	-	34,36,36	0.99	1 (2%)	46,53,53	2.13	10 (21%)
3	NAG	B	1085	1	14,14,15	0.49	0	15,19,21	1.70	1 (6%)
3	NAG	B	1150	1	14,14,15	0.50	0	15,19,21	1.42	1 (6%)
3	NAG	B	1281	1	14,14,15	0.56	0	15,19,21	1.40	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	W61	A	1000	-	-	0/22/48/48	0/5/5/5
3	NAG	A	1085	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1092	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1229	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1321	1	-	0/6/23/26	0/1/1/1
2	W61	B	1000	-	-	0/22/48/48	0/5/5/5
3	NAG	B	1085	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1150	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1281	1	-	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)
2	B	1000	W61	C3-N4	3.31	1.34	1.31
2	A	1000	W61	C3-N4	4.17	1.35	1.31

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	W61	C2-C3-N4	-8.80	120.59	125.50
2	B	1000	W61	C2-C3-N4	-8.18	120.94	125.50
2	B	1000	W61	F53-C11-C3	-3.58	106.20	112.55
2	A	1000	W61	F52-C11-C3	-3.44	106.46	112.55
2	B	1000	W61	C6-C5-N4	-2.59	120.37	122.90
2	A	1000	W61	C6-C5-N4	-2.49	120.47	122.90
2	A	1000	W61	F54-C11-C3	-2.15	108.73	112.55
3	A	1092	NAG	C6-C5-C4	-2.03	108.01	113.02
3	A	1092	NAG	O7-C7-C8	-2.01	118.37	122.06
2	A	1000	W61	C49-C50-N46	2.21	111.79	106.82
2	A	1000	W61	C10-C5-C6	2.22	121.58	119.07
2	B	1000	W61	C6-C1-N20	2.34	123.30	118.91
3	A	1321	NAG	C3-C2-N2	2.39	116.29	110.56
2	A	1000	W61	C49-S48-C47	2.50	98.28	91.83
3	B	1281	NAG	O5-C5-C6	2.67	113.14	107.35
3	A	1092	NAG	C3-C4-C5	2.74	114.97	110.20
2	B	1000	W61	C49-S48-C47	2.77	98.97	91.83
2	B	1000	W61	C10-C5-C6	2.79	122.22	119.07
2	B	1000	W61	C2-C3-C11	3.06	123.27	119.91
3	A	1092	NAG	C8-C7-N2	3.09	122.01	116.11
2	A	1000	W61	C24-N23-C22	3.28	115.19	109.23
3	B	1281	NAG	C1-O5-C5	3.79	117.06	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	W61	C24-N23-C22	3.80	116.12	109.23
3	A	1229	NAG	C1-O5-C5	3.86	117.15	112.25
3	B	1150	NAG	C1-O5-C5	3.93	117.24	112.25
2	B	1000	W61	C1-C6-C5	4.25	120.04	116.58
2	A	1000	W61	C2-C3-C11	4.46	124.81	119.91
2	A	1000	W61	C1-C6-C5	4.47	120.22	116.58
2	A	1000	W61	C3-N4-C5	5.18	121.30	117.30
2	B	1000	W61	C3-N4-C5	5.27	121.36	117.30
3	A	1092	NAG	C1-O5-C5	5.34	119.03	112.25
3	A	1092	NAG	C2-N2-C7	5.42	130.00	123.04
3	A	1321	NAG	C1-O5-C5	5.92	119.76	112.25
3	B	1085	NAG	C1-O5-C5	5.94	119.78	112.25
3	A	1085	NAG	C1-O5-C5	7.95	122.33	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	W61	3	0
3	A	1092	NAG	1	0
3	A	1229	NAG	1	0
2	B	1000	W61	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	729/740 (98%)	-0.16	19 (2%) 59 66	16, 26, 45, 64	0
1	B	729/740 (98%)	-0.23	18 (2%) 61 67	16, 25, 46, 57	0
All	All	1458/1480 (98%)	-0.20	37 (2%) 61 67	16, 26, 46, 64	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	LEU	11.4
1	A	766	PRO	10.4
1	B	766	PRO	9.2
1	B	765	LEU	6.2
1	A	138	ASN	4.5
1	B	279	VAL	4.0
1	B	97	GLU	4.0
1	B	74	ASN	3.6
1	B	140	ARG	3.4
1	A	39	SER	3.3
1	A	97	GLU	3.2
1	B	105	TYR	3.0
1	B	505	GLN	2.9
1	A	333	SER	2.7
1	A	505	GLN	2.7
1	A	96	ASP	2.6
1	A	73	GLU	2.6
1	A	100	HIS	2.6
1	A	502	LYS	2.6
1	B	521	GLU	2.5
1	B	138	ASN	2.5
1	B	506	ASN	2.5
1	A	676	PRO	2.4
1	B	73	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	98	PHE	2.4
1	B	92	ASN	2.4
1	B	333	SER	2.4
1	A	521	GLU	2.3
1	A	91	GLU	2.3
1	B	543	LEU	2.2
1	A	140	ARG	2.2
1	B	96	ASP	2.1
1	A	506	ASN	2.1
1	B	137	LEU	2.1
1	A	653	VAL	2.1
1	A	764	SER	2.0
1	B	93	SER	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	B	1219	14/15	0.87	0.17	4.38	45,51,53,54	0
4	NAG	B	1321	14/15	0.87	0.17	3.81	42,47,51,52	0
4	NAG	A	1219	14/15	0.93	0.17	3.02	38,42,45,45	0
4	NAG	A	1220	14/15	0.87	0.27	2.79	48,50,52,52	0
4	NAG	B	1220	14/15	0.79	0.27	2.21	56,60,62,63	0
4	NAG	A	1281	14/15	0.96	0.10	-0.02	24,26,30,32	0
4	NAG	B	1229	14/15	0.94	0.11	-0.06	36,41,45,49	0
4	NAG	A	1282	14/15	0.92	0.09	-	32,34,36,38	0
4	NAG	B	1230	14/15	0.83	0.27	-	53,56,58,60	0
4	NAG	B	1322	14/15	0.73	0.33	-	55,57,58,59	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	1321	14/15	0.81	0.20	2.63	36,39,42,42	0
3	NAG	B	1085	14/15	0.89	0.15	1.35	40,43,46,46	0
3	NAG	A	1085	14/15	0.88	0.14	1.10	47,49,52,54	0
3	NAG	A	1229	14/15	0.91	0.14	0.98	29,33,38,39	0
2	W61	A	1000	32/32	0.94	0.10	-0.07	17,24,39,41	0
2	W61	B	1000	32/32	0.96	0.09	-0.45	18,26,39,40	0
3	NAG	A	1092	14/15	0.68	0.32	-	69,71,74,75	0
3	NAG	B	1281	14/15	0.77	0.18	-	50,52,52,53	0
3	NAG	B	1150	14/15	0.86	0.23	-	48,51,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.