



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:21 PM GMT

PDB ID : 1X70  
Title : HUMAN DIPEPTIDYL PEPTIDASE IV IN COMPLEX WITH A BETA AMINO ACID INHIBITOR  
Authors : Kim, D.; Wang, L.; Beconi, M.; Eiermann, G.J.; Fisher, M.H.; He, H.; Hickey, G.J.; Leiting, B.; Lyons, K.  
Deposited on : 2004-08-12  
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

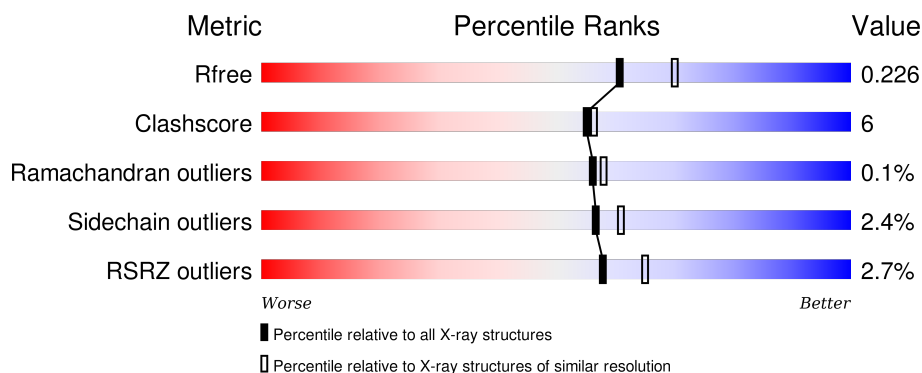
# 1 Overall quality at a glance

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	728	 2% 85% 14%
1	B	728	 4% 84% 14%

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	B	2321	-	-	-	X
5	NAG	A	1219	-	-	-	X
5	NAG	A	1321	-	-	-	X
5	NAG	B	2219	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13430 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	728	Total	C	N	O	S	0	3	0
			5984	3839	985	1134	26			
1	B	728	Total	C	N	O	S	0	6	0
			6005	3850	989	1138	28			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

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

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

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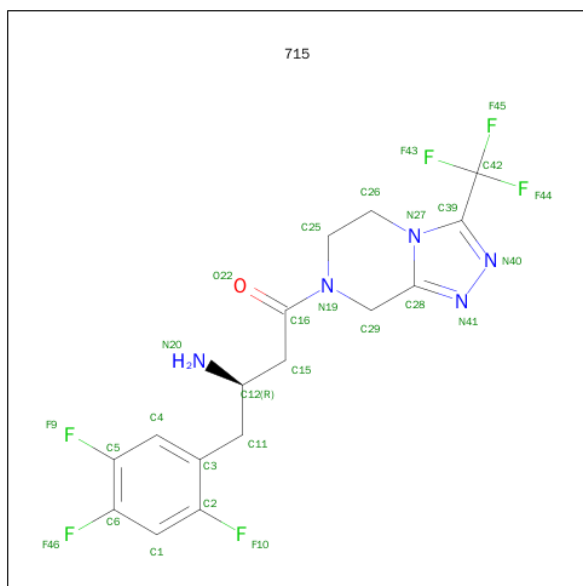
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is (2R)-4-OXO-4-[3-(TRIFLUOROMETHYL)-5,6-DIHYDRO[1,2,4]TRIAZOLO[4,3-A]PYRAZIN-7(8H)-YL]-1-(2,4,5-TRIFLUOROPHENYL)BUTAN-2-AMINE (three-letter code: 715) (formula: C<sub>16</sub>H<sub>15</sub>F<sub>6</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			28	16	6	5	1		
7	B	1	Total	C	F	N	O	0	0
			28	16	6	5	1		

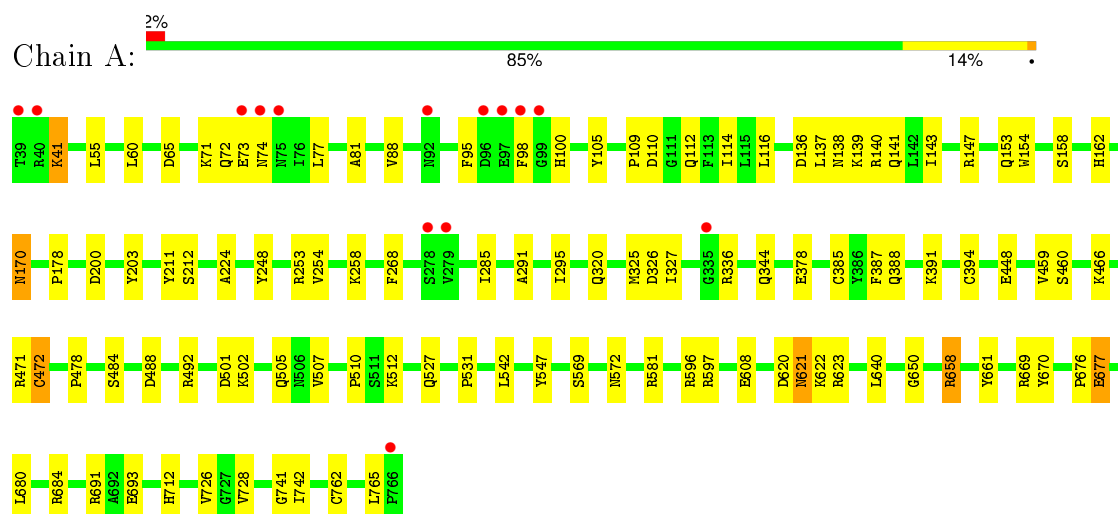
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	537	Total 537	O 537	0	0
8	B	511	Total 511	O 511	0	0

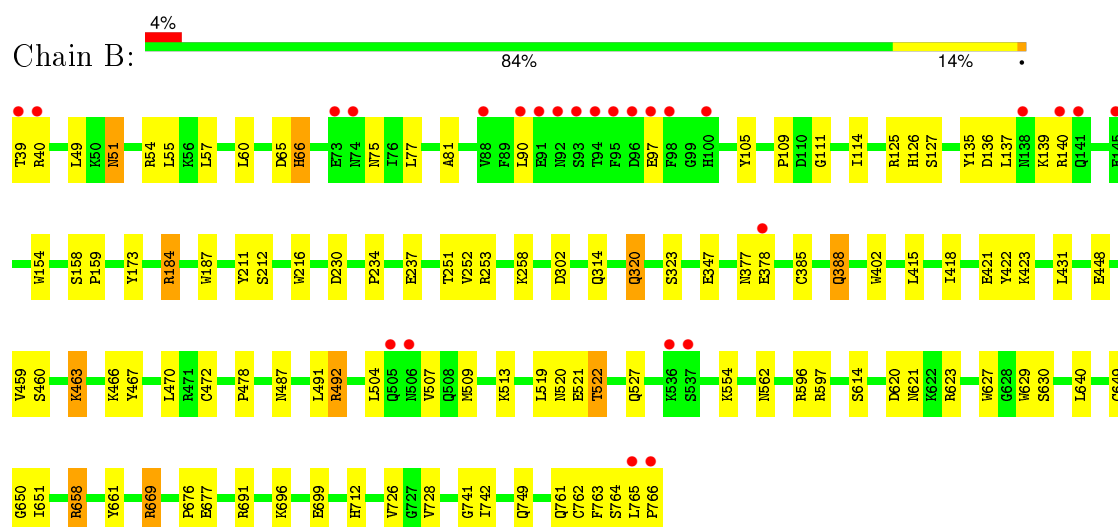
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Dipeptidyl peptidase IV





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.25Å 125.68Å 137.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 46.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.10) 99.8 (46.34-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.75 (at 2.10Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.193 , 0.228 0.191 , 0.226	Depositor DCC
$R_{free}$ test set	6018 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 119323 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: NA, 715, NAG, NDG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	0/6156	0.68	0/8372
1	B	0.46	0/6177	0.68	2/8401 (0.0%)
All	All	0.46	0/12333	0.68	2/16773 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	669	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	388	GLN	N-CA-C	-5.50	96.16	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	TYR	Sidechain

### 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	5984	0	5692	74	0
1	B	6005	0	5708	77	0
2	A	56	0	50	1	0
3	A	42	0	39	5	0
3	B	42	0	39	1	0
4	A	28	0	25	0	0
5	A	56	0	50	1	0
5	B	112	0	100	0	0
6	A	1	0	0	0	0
7	A	28	0	15	2	0
7	B	28	0	15	0	0
8	A	537	0	0	7	0
8	B	511	0	0	7	0
All	All	13430	0	11733	152	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 6.

All (152) 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:762:CYS:HB2	8:A:1533:HOH:O	1.68	0.92
1:A:596:ARG:O	1:A:597:ARG:HD2	1.78	0.81
1:B:649[B]:CYS:SG	1:B:699:GLU:HB2	2.21	0.80
1:A:581:ARG:CZ	3:A:1520:NAG:H62	2.12	0.78
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.64	0.78
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.84	0.76
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.86	0.75
1:B:173:TYR:CE2	1:B:184:ARG:HG2	2.23	0.74
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.36	0.74
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.69	0.72
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.92	0.68
1:B:378:GLU:HG2	8:B:2542:HOH:O	1.93	0.67
1:B:614:SER:HB2	1:B:621:ASN:OD1	1.96	0.66
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.94	0.65
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.26	0.65
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.34	0.62
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.18	0.62
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ARG:HD2	8:B:2345:HOH:O	2.01	0.60
1:B:596:ARG:O	1:B:597:ARG:HD2	2.01	0.60
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.82	0.60
1:A:501:ASP:O	1:A:505:GLN:HG3	2.02	0.59
1:B:39:THR:O	1:B:40:ARG:HB2	2.02	0.59
1:B:51[A]:ASN:OD1	1:B:54:ARG:HD3	2.03	0.59
1:A:581:ARG:NH1	3:A:1520:NAG:H62	2.17	0.58
1:B:323[A]:SER:OG	1:B:347:GLU:HB3	2.03	0.58
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.84	0.58
1:A:291:ALA:O	1:A:295:ILE:HG23	2.05	0.57
1:A:378:GLU:HG2	8:A:1628:HOH:O	2.05	0.57
1:A:139:LYS:HG3	1:A:141:GLN:HB2	1.87	0.56
1:B:109:PRO:HG2	1:B:158:SER:O	2.06	0.56
1:A:621:ASN:HD22	1:A:622:LYS:N	2.03	0.56
1:B:422:TYR:CE2	1:B:423:LYS:HE2	2.41	0.56
1:B:764:SER:C	1:B:766:PRO:HD3	2.26	0.55
1:A:621:ASN:C	1:A:621:ASN:HD22	2.10	0.55
1:A:170:ASN:N	1:A:170:ASN:HD22	2.05	0.55
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.87	0.55
1:B:507:VAL:HG13	1:B:509:MET:HG2	1.89	0.55
1:B:520:ASN:O	1:B:521:GLU:HB2	2.06	0.54
1:B:184:ARG:NH1	1:B:187:TRP:HA	2.21	0.54
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.28	0.53
1:B:75:ASN:HD21	3:B:2092:NAG:C1	2.21	0.53
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.91	0.53
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.89	0.53
1:B:60:LEU:HD12	1:B:60:LEU:C	2.28	0.53
1:A:691:ARG:HD2	8:A:1531:HOH:O	2.09	0.53
1:A:258:LYS:HZ3	1:A:712:HIS:HD2	1.57	0.52
1:B:658:ARG:HG3	1:B:658:ARG:O	2.09	0.52
1:A:253:ARG:HH21	1:B:253:ARG:NH2	2.07	0.52
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.45	0.52
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.10	0.52
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.44	0.52
5:A:1321:NAG:H61	5:A:1322:NAG:O5	2.10	0.51
1:B:463:LYS:HE3	1:B:463:LYS:HA	1.93	0.51
1:B:81:ALA:O	1:B:492:ARG:NH2	2.42	0.51
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.93	0.51
1:A:693:GLU:HG3	1:A:726:VAL:HG11	1.92	0.51
1:A:41:LYS:HD3	1:A:41:LYS:H	1.76	0.50
1:B:111:GLY:O	1:B:137:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.32	0.50
1:A:253:ARG:HH21	1:B:253:ARG:CZ	2.25	0.50
1:B:323[A]:SER:HG	1:B:347:GLU:HB3	1.75	0.49
1:B:251:THR:HG21	1:B:253:ARG:NH1	2.26	0.49
1:B:763:PHE:HB3	1:B:765:LEU:HD23	1.94	0.49
1:A:81:ALA:O	1:A:492:ARG:NH2	2.34	0.49
1:B:741:GLY:O	1:B:742:ILE:C	2.50	0.49
1:B:554:LYS:HG2	8:B:2409:HOH:O	2.11	0.49
1:A:387:PHE:CD1	1:A:394:CYS:HB3	2.47	0.49
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.58	0.49
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.95	0.49
1:B:66:HIS:HB3	1:B:467:TYR:HE2	1.77	0.48
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.43	0.48
1:B:415:LEU:HD23	1:B:415:LEU:C	2.33	0.48
1:B:388:GLN:HG3	8:B:2665:HOH:O	2.13	0.48
1:B:77:LEU:HD12	1:B:77:LEU:N	2.28	0.48
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.48	0.48
1:B:519:LEU:O	1:B:522:THR:HG23	2.13	0.48
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.49	0.47
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.49	0.47
1:A:547:TYR:HB3	8:A:1994:HOH:O	2.13	0.47
1:A:143:ILE:CD1	1:A:178:PRO:HB2	2.45	0.47
1:A:620:ASP:OD2	1:A:623:ARG:HD3	2.13	0.47
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.50	0.47
1:A:73:GLU:O	1:A:74:ASN:HB2	2.13	0.46
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.16	0.46
1:A:502:LYS:HB2	1:A:502:LYS:NZ	2.31	0.46
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.50	0.46
1:A:41:LYS:HE2	1:A:507:VAL:HG22	1.98	0.45
1:B:629:TRP:O	1:B:630:SER:HB3	2.14	0.45
1:A:73:GLU:HB3	3:A:1092:NAG:HN2	1.81	0.45
1:A:512:LYS:HD3	8:A:1839:HOH:O	2.16	0.45
1:A:391:LYS:HG3	8:A:1608:HOH:O	2.17	0.45
1:A:137:LEU:O	1:A:140:ARG:HD2	2.17	0.45
1:B:55:LEU:HD11	1:B:478:PRO:HD2	1.98	0.45
1:B:459:VAL:HG22	1:B:460:SER:N	2.32	0.45
2:A:1085:NAG:O3	2:A:1086:NDG:O	2.32	0.44
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.98	0.44
1:B:470:LEU:HD23	1:B:470:LEU:HA	1.84	0.44
7:A:801:715:H262	8:A:1551:HOH:O	2.17	0.44
1:B:491:LEU:O	1:B:492:ARG:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LYS:O	1:B:527:GLN:HA	2.18	0.44
1:A:110:ASP:OD1	1:A:162:HIS:HD2	2.01	0.44
1:A:512:LYS:HE3	1:A:527:GLN:OE1	2.18	0.44
7:A:801:715:H252	7:A:801:715:H152	1.63	0.44
1:B:237:GLU:CD	1:B:253:ARG:HH11	2.21	0.43
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.62	0.43
1:B:60:LEU:HD12	1:B:60:LEU:O	2.18	0.43
1:B:676:PRO:HG2	1:B:677:GLU:OE1	2.18	0.43
1:A:285:ILE:HG23	1:A:336:ARG:HE	1.84	0.43
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.48	0.43
1:A:459:VAL:HG22	1:A:460:SER:N	2.33	0.43
1:A:109:PRO:HG2	1:A:158:SER:O	2.18	0.43
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.54	0.43
1:A:200:ASP:OD1	1:A:203:TYR:HB2	2.18	0.43
1:A:387:PHE:CE1	1:A:394:CYS:HB3	2.53	0.43
1:A:72:GLN:O	1:A:73:GLU:HB2	2.18	0.43
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.54	0.43
1:A:73:GLU:O	3:A:1092:NAG:C1	2.67	0.43
1:A:472:CYS:O	1:A:478:PRO:HA	2.19	0.43
1:B:763:PHE:CB	1:B:765:LEU:HD23	2.49	0.42
1:B:418:ILE:HD13	1:B:431:LEU:HA	2.01	0.42
1:A:484:SER:O	1:A:488:ASP:HA	2.20	0.42
1:A:741:GLY:O	1:A:742:ILE:C	2.57	0.42
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.55	0.42
1:A:621:ASN:ND2	1:A:621:ASN:C	2.72	0.42
1:B:521:GLU:OE2	1:B:521:GLU:HA	2.20	0.42
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.01	0.42
1:B:49:LEU:HD22	1:B:749:GLN:HA	2.02	0.42
1:B:125:ARG:HG2	1:B:126:HIS:CD2	2.55	0.41
1:A:623:ARG:NH2	1:A:765:LEU:HD21	2.35	0.41
1:A:95:PHE:CE1	1:A:116:LEU:HD11	2.55	0.41
1:A:676:PRO:HG2	1:A:677:GLU:OE2	2.20	0.41
1:B:377:ASN:HB2	8:B:2542:HOH:O	2.19	0.41
1:B:90:LEU:HA	1:B:90:LEU:HD12	1.93	0.41
1:A:60:LEU:HD12	1:A:60:LEU:C	2.40	0.41
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.20	0.41
1:A:55:LEU:HD23	1:A:478:PRO:HG2	2.02	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.20	0.41
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.85	0.41
1:B:562:ASN:HB2	8:B:2408:HOH:O	2.21	0.41
1:A:677:GLU:H	1:A:677:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:O	1:B:507:VAL:HG12	2.20	0.41
1:A:71:LYS:HZ3	1:A:74:ASN:HA	1.86	0.41
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.02	0.41
1:A:112:GLN:HB3	1:A:138:ASN:HD21	1.85	0.41
1:B:66:HIS:HB2	8:B:2766:HOH:O	2.20	0.41
1:A:542:LEU:HD23	1:A:542:LEU:C	2.41	0.41
1:B:699:GLU:OE1	1:B:762[B]:CYS:SG	2.79	0.40
1:A:726:VAL:HG23	1:A:728:VAL:HG23	2.02	0.40
1:A:336:ARG:HH11	1:A:336:ARG:HG3	1.85	0.40
1:A:581:ARG:NH2	3:A:1520:NAG:H62	2.33	0.40
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.67	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	729/728 (100%)	704 (97%)	24 (3%)	1 (0%)	56	58
1	B	732/728 (100%)	701 (96%)	30 (4%)	1 (0%)	56	58
All	All	1461/1456 (100%)	1405 (96%)	54 (4%)	2 (0%)	56	58

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	656/653 (100%)	641 (98%)	15 (2%)	58	62
1	B	659/653 (101%)	642 (97%)	17 (3%)	54	58
All	All	1315/1306 (101%)	1283 (98%)	32 (2%)	57	61

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	147	ARG
1	A	170	ASN
1	A	254	VAL
1	A	326	ASP
1	A	344	GLN
1	A	385	CYS
1	A	388	GLN
1	A	448	GLU
1	A	471	ARG
1	A	472	CYS
1	A	608	GLU
1	A	621	ASN
1	A	658	ARG
1	A	677	GLU
1	B	51[A]	ASN
1	B	51[B]	ASN
1	B	57	LEU
1	B	66	HIS
1	B	97	GLU
1	B	140	ARG
1	B	184	ARG
1	B	230	ASP
1	B	385	CYS
1	B	448	GLU
1	B	463	LYS
1	B	472	CYS

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Mol	Chain	Res	Type
1	B	487	ASN
1	B	492	ARG
1	B	522	THR
1	B	658	ARG
1	B	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	123	GLN
1	A	138	ASN
1	A	162	HIS
1	A	169	ASN
1	A	170	ASN
1	A	363	HIS
1	A	430	ASN
1	A	435	GLN
1	A	572	ASN
1	A	621	ASN
1	A	712	HIS
1	B	141	GLN
1	B	169	ASN
1	B	314	GLN
1	B	345	HIS
1	B	435	GLN
1	B	487	ASN
1	B	505	GLN
1	B	712	HIS
1	B	761	GLN

### 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

18 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	1085	1,2	14,14,15	0.76	0	15,19,21	1.25	3 (20%)
2	NDG	A	1086	2	14,14,15	0.72	0	15,19,21	0.78	1 (6%)
4	NDG	A	1150	1,4	14,14,15	0.75	1 (7%)	15,19,21	0.92	0
4	NAG	A	1151	4	14,14,15	0.66	0	15,19,21	0.62	0
5	NAG	A	1219	1,5	14,14,15	0.52	0	15,19,21	0.93	1 (6%)
5	NAG	A	1220	5	14,14,15	0.61	0	15,19,21	0.75	0
2	NAG	A	1229	1,2	14,14,15	0.57	0	15,19,21	0.72	0
2	NDG	A	1230	2	14,14,15	0.82	0	15,19,21	1.17	1 (6%)
5	NAG	A	1321	1,5	14,14,15	0.71	0	15,19,21	0.95	1 (6%)
5	NAG	A	1322	5	14,14,15	0.56	0	15,19,21	0.66	0
5	NAG	B	2085	1,5	14,14,15	0.70	0	15,19,21	1.05	1 (6%)
5	NAG	B	2086	5	14,14,15	0.63	0	15,19,21	0.57	0
5	NAG	B	2219	1,5	14,14,15	0.59	0	15,19,21	0.63	0
5	NAG	B	2220	5	14,14,15	0.56	0	15,19,21	0.65	0
5	NAG	B	2229	1,5	14,14,15	0.51	0	15,19,21	0.84	0
5	NAG	B	2230	5	14,14,15	0.61	0	15,19,21	0.83	1 (6%)
5	NAG	B	2281	1,5	14,14,15	0.40	0	15,19,21	0.97	1 (6%)
5	NAG	B	2282	5	14,14,15	0.54	0	15,19,21	0.87	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	1085	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	1086	2	-	0/6/23/26	0/1/1/1
4	NDG	A	1150	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1151	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1219	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1220	5	-	0/6/23/26	0/1/1/1
2	NAG	A	1229	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	1230	2	-	0/6/23/26	0/1/1/1
5	NAG	A	1321	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1322	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2085	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2086	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2219	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2220	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2229	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2230	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2281	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2282	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1150	NDG	C1-C2	2.33	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1219	NAG	C2-N2-C7	-3.00	119.19	123.04
2	A	1085	NAG	C4-C3-C2	-2.88	106.76	111.23
5	B	2230	NAG	C2-N2-C7	-2.75	119.50	123.04
5	B	2281	NAG	C2-N2-C7	-2.73	119.53	123.04
5	B	2282	NAG	C2-N2-C7	-2.58	119.72	123.04
2	A	1085	NAG	C2-N2-C7	-2.47	119.86	123.04
2	A	1086	NDG	C2-N2-C7	-2.37	119.99	123.04
5	A	1321	NAG	C2-N2-C7	-2.31	120.07	123.04
2	A	1085	NAG	O4-C4-C3	2.14	115.15	110.34
5	B	2085	NAG	C4-C3-C2	2.85	115.66	111.23
2	A	1230	NDG	C4-C3-C2	3.59	116.81	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1085	NAG	1	0
2	A	1086	NDG	1	0
5	A	1321	NAG	1	0
5	A	1322	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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$
3	NAG	A	1092	1	14,14,15	0.79	1 (7%)	15,19,21	0.56	0
3	NAG	A	1281	1	14,14,15	0.68	0	15,19,21	0.86	1 (6%)
3	NAG	A	1520	1	14,14,15	0.64	0	15,19,21	0.70	0
7	715	A	801	-	28,30,30	2.51	11 (39%)	28,45,45	2.28	8 (28%)
3	NAG	B	2092	1	14,14,15	0.64	0	15,19,21	0.71	0
3	NAG	B	2150	1	14,14,15	0.60	0	15,19,21	0.69	1 (6%)
3	NAG	B	2321	1	14,14,15	0.54	0	15,19,21	1.20	2 (13%)
7	715	B	801	-	28,30,30	2.61	11 (39%)	28,45,45	2.29	9 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1092	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1281	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1520	1	-	0/6/23/26	0/1/1/1
7	715	A	801	-	-	0/18/27/27	0/2/3/3
3	NAG	B	2092	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2150	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2321	1	-	0/6/23/26	0/1/1/1
7	715	B	801	-	-	0/18/27/27	0/2/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	801	715	N41-N40	-5.73	1.26	1.37
7	A	801	715	N41-N40	-5.46	1.26	1.37
7	B	801	715	F46-C6	-3.13	1.28	1.35
7	A	801	715	F46-C6	-2.01	1.30	1.35
3	A	1092	NAG	C1-C2	2.17	1.55	1.52
7	B	801	715	C29-C28	2.29	1.55	1.51
7	A	801	715	C42-C39	2.42	1.53	1.51
7	A	801	715	C4-C3	2.59	1.44	1.39
7	A	801	715	C1-C6	2.69	1.42	1.37
7	B	801	715	C4-C5	2.70	1.42	1.37
7	B	801	715	C1-C6	2.81	1.42	1.37
7	A	801	715	C1-C2	3.12	1.43	1.37
7	B	801	715	C4-C3	3.25	1.45	1.39
7	B	801	715	C1-C2	3.41	1.43	1.37
7	A	801	715	C4-C5	3.48	1.43	1.37
7	A	801	715	C3-C2	3.65	1.44	1.38
7	B	801	715	C15-C16	3.73	1.58	1.51
7	A	801	715	C16-N19	3.96	1.44	1.35
7	B	801	715	C3-C2	4.00	1.45	1.38
7	B	801	715	C16-N19	4.21	1.44	1.35
7	A	801	715	C15-C16	4.46	1.59	1.51
7	A	801	715	C29-N19	6.05	1.56	1.46
7	B	801	715	C29-N19	6.47	1.57	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	801	715	C25-N19-C16	-4.88	107.69	122.77
7	A	801	715	C25-N19-C16	-4.73	108.18	122.77
7	A	801	715	F44-C42-C39	-4.17	106.85	111.32
7	A	801	715	F43-C42-C39	-3.24	107.84	111.32
7	B	801	715	F44-C42-C39	-3.22	107.86	111.32
7	B	801	715	F43-C42-C39	-3.13	107.97	111.32
7	B	801	715	F45-C42-C39	-2.89	108.21	111.32
3	B	2321	NAG	C2-N2-C7	-2.87	119.35	123.04
3	B	2321	NAG	C4-C3-C2	-2.56	107.25	111.23
3	A	1281	NAG	C2-N2-C7	-2.30	120.08	123.04
3	B	2150	NAG	C2-N2-C7	-2.30	120.09	123.04
7	A	801	715	C11-C12-C15	-2.26	106.96	110.81
7	B	801	715	O22-C16-C15	-2.15	118.08	122.22
7	A	801	715	C4-C3-C2	2.42	118.40	116.52
7	B	801	715	C42-C39-N27	2.55	126.71	124.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	801	715	C42-C39-N27	2.60	126.75	124.19
7	B	801	715	C4-C3-C2	2.86	118.75	116.52
7	A	801	715	C26-N27-C39	4.43	131.42	125.73
7	B	801	715	C26-N27-C39	4.81	131.91	125.73
7	B	801	715	C26-C25-N19	5.52	116.75	110.48
7	A	801	715	C26-C25-N19	5.85	117.12	110.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1092	NAG	2	0
3	A	1520	NAG	3	0
7	A	801	715	2	0
3	B	2092	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<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	728/728 (100%)	-0.02	14 (1%) 70 75	14, 24, 42, 54	0
1	B	728/728 (100%)	0.02	26 (3%) 46 55	15, 26, 44, 54	0
All	All	1456/1456 (100%)	0.00	40 (2%) 58 65	14, 25, 43, 54	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	766	PRO	7.3
1	A	39	THR	7.1
1	B	39	THR	5.8
1	A	766	PRO	5.6
1	A	92	ASN	4.6
1	B	92	ASN	4.6
1	A	97	GLU	4.4
1	B	96	ASP	4.3
1	A	74	ASN	4.0
1	B	91	GLU	3.8
1	B	93	SER	3.7
1	B	765	LEU	3.7
1	A	96	ASP	3.5
1	B	74	ASN	3.3
1	B	73	GLU	3.3
1	B	97	GLU	3.2
1	A	278	SER	3.1
1	B	40	ARG	3.1
1	A	73	GLU	3.1
1	B	95	PHE	3.1
1	B	88	VAL	2.9
1	B	505	GLN	2.9
1	A	40	ARG	2.8
1	B	94	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	98	PHE	2.7
1	A	279	VAL	2.6
1	B	140	ARG	2.6
1	B	536	LYS	2.5
1	A	75	ASN	2.5
1	A	99	GLY	2.5
1	B	138	ASN	2.5
1	A	98	PHE	2.4
1	B	506	ASN	2.4
1	A	335	GLY	2.3
1	B	100	HIS	2.3
1	B	90	LEU	2.2
1	B	378	GLU	2.1
1	B	145	GLU	2.1
1	B	537	SER	2.1
1	B	141	GLN	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( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	1321	14/15	0.72	0.26	6.66	38,42,44,49	0
5	NAG	A	1219	14/15	0.88	0.17	2.69	37,41,44,44	0
5	NAG	B	2219	14/15	0.91	0.13	2.68	34,39,42,42	0
2	NAG	A	1085	14/15	0.88	0.16	1.98	43,44,49,51	0
5	NAG	B	2085	14/15	0.82	0.22	1.96	43,47,51,53	0
5	NAG	A	1220	14/15	0.84	0.25	1.78	46,48,52,52	0
2	NAG	A	1229	14/15	0.90	0.14	0.96	33,35,44,44	0
5	NAG	B	2281	14/15	0.92	0.11	0.95	32,34,38,41	0
5	NAG	B	2220	14/15	0.90	0.15	0.43	43,44,45,46	0
5	NAG	B	2229	14/15	0.92	0.12	0.19	26,31,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	2282	14/15	0.64	0.24	-	43,46,47,47	0
4	NAG	A	1151	14/15	0.60	0.45	-	56,57,59,59	0
5	NAG	B	2230	14/15	0.84	0.28	-	43,46,48,48	0
2	NDG	A	1230	14/15	0.60	0.37	-	48,52,54,54	0
5	NAG	B	2086	14/15	0.41	0.47	-	54,55,57,57	0
5	NAG	A	1322	14/15	0.56	0.36	-	51,53,55,56	0
4	NDG	A	1150	14/15	0.68	0.32	-	47,50,53,54	0
2	NDG	A	1086	14/15	0.67	0.33	-	53,54,55,55	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	2321	14/15	0.82	0.22	4.50	37,42,44,44	0
7	715	A	801	28/28	0.89	0.17	0.62	19,26,37,39	0
7	715	B	801	28/28	0.89	0.16	0.59	18,26,39,40	0
6	NA	A	1200	1/1	0.95	0.08	-1.73	26,26,26,26	0
3	NAG	A	1281	14/15	0.86	0.14	-	41,43,44,45	0
3	NAG	A	1520	14/15	0.66	0.39	-	54,55,57,57	0
3	NAG	B	2092	14/15	0.69	0.43	-	54,55,55,56	0
3	NAG	B	2150	14/15	0.82	0.33	-	46,48,50,50	0
3	NAG	A	1092	14/15	0.58	0.52	-	58,58,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.