



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:48 am GMT

PDB ID : 3HAC
Title : The structure of DPP-4 in complex with piperidine fused imidazopyridine 34
Authors : Scapin, G.
Deposited on : 2009-05-01
Resolution : 2.00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

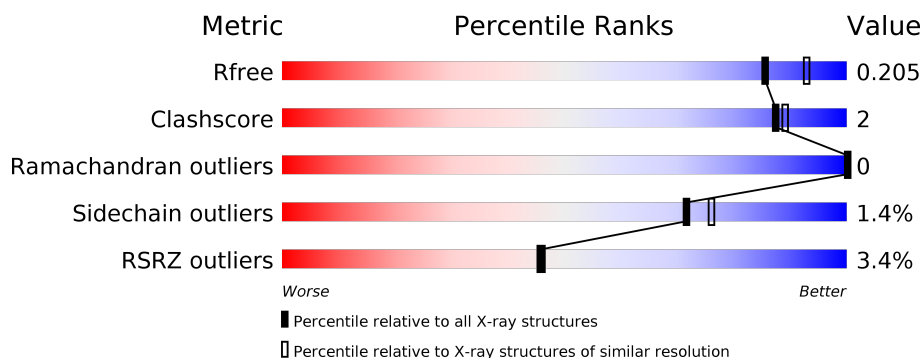
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 $\leq 5\%$. 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	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	728	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>7%</div> </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
2	NAG	A	1085	-	-	-	X
3	NAG	A	1219	-	-	-	X
3	NAG	A	1220	-	-	-	X
3	NAG	A	1321	-	-	-	X
3	NAG	B	2085	-	-	-	X
3	NAG	B	2219	-	-	-	X
3	NAG	B	2220	-	-	-	X
4	NAG	B	2321	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13578 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	12	0
			6015	3862	990	1136	27			
1	B	728	Total	C	N	O	S	0	10	0
			6002	3849	987	1139	27			

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 (2-MER).

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

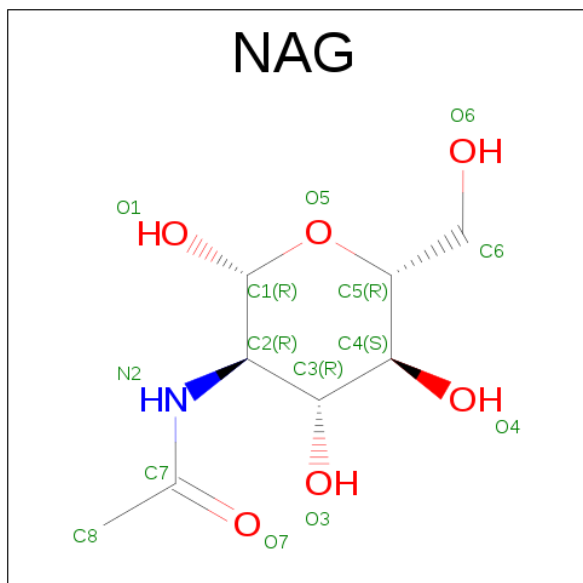
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

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

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

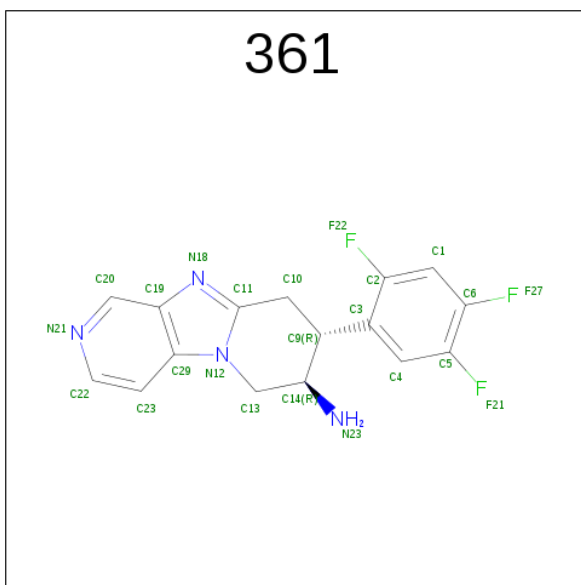


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

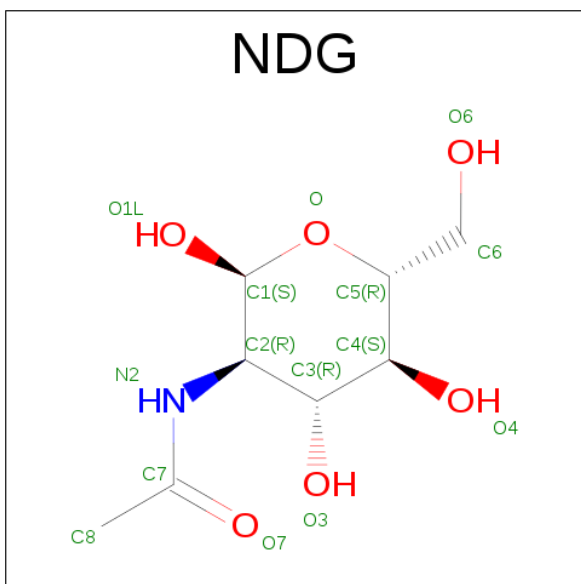
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is (7R,8R)-8-(2,4,5-TRIFLUOROPHENYL)-6,7,8,9-TETRAHYDROIMIDAZO[1,2-A:4,5-C']DIPYRIDIN-7-AMINE (three-letter code: 361) (formula: $C_{16}H_{13}F_3N_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	F	N	0	0
			23	16	3	4		
6	B	1	Total	C	F	N	0	0
			23	16	3	4		

- Molecule 7 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (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		

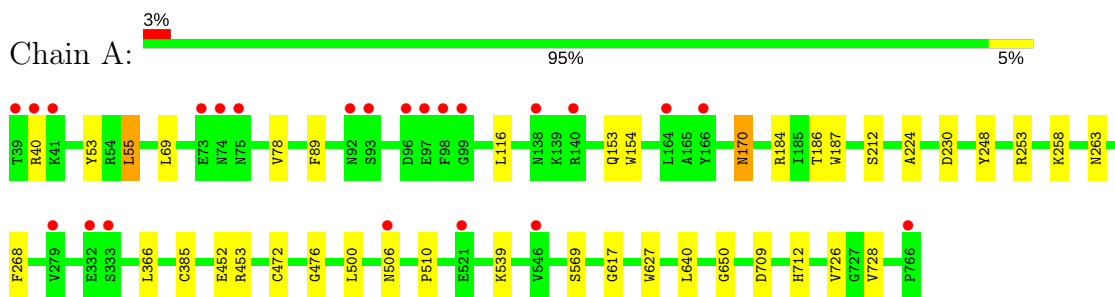
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	615	Total 615	O 615	0	0
8	B	591	Total 591	O 591	0	0

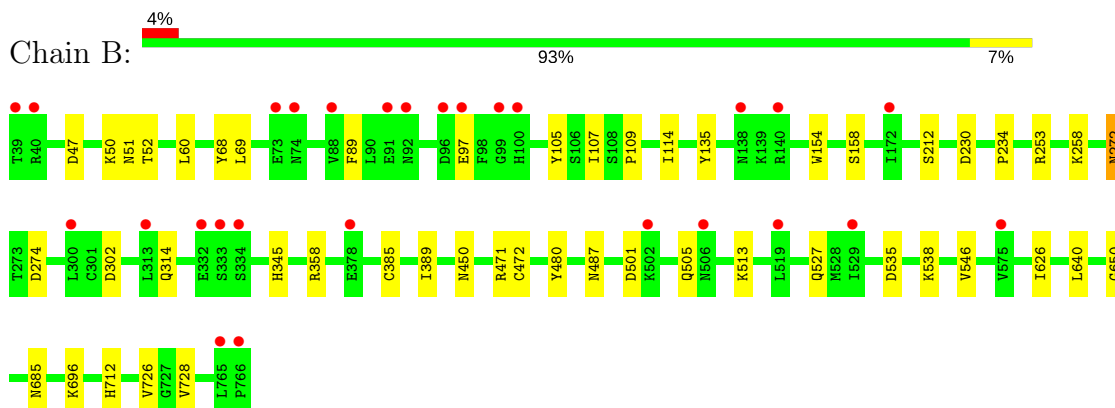
3 Residue-property plots [i](#)

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

• Molecule 1: Dipeptidyl peptidase 4



• 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, α , β , γ	118.12Å 125.50Å 136.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.00) 99.7 (29.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.171 , 0.205 0.172 , 0.205	Depositor DCC
R_{free} test set	6880 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13578	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, NAG, NDG, 361

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	0.56	0/6236	0.61	0/8478
1	B	0.54	0/6214	0.59	0/8451
All	All	0.55	0/12450	0.60	0/16929

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	6015	0	5731	27	0
1	B	6002	0	5706	31	0
2	A	56	0	50	0	0
3	A	84	0	75	2	0
3	B	112	0	100	1	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
5	A	1	0	0	0	0
6	A	23	0	13	0	0
6	B	23	0	13	0	0
7	B	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	615	0	0	2	0
8	B	591	0	0	3	0
All	All	13578	0	11740	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (59) 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:69:LEU:HD23	1:A:78:VAL:HG22	1.45	0.97
1:B:69:LEU:HD11	1:B:107:ILE:HD12	1.60	0.83
1:A:184:ARG:HD2	1:A:186:THR:O	1.83	0.79
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.16	0.75
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.92	0.68
1:A:69:LEU:HD23	1:A:78:VAL:CG2	2.21	0.67
1:A:69:LEU:CD2	1:A:78:VAL:HG22	2.21	0.67
1:A:452[A]:GLU:HG2	8:A:877:HOH:O	1.95	0.66
1:B:47:ASP:HA	1:B:52[B]:THR:CG2	2.27	0.64
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.98	0.61
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.49	0.60
1:B:272:ASN:C	1:B:272:ASN:HD22	2.04	0.60
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.68	0.59
1:A:184:ARG:HG2	1:A:187:TRP:CE2	2.37	0.58
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.86	0.58
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.85	0.58
1:A:69:LEU:CD2	1:A:78:VAL:CG2	2.83	0.56
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.54	0.56
1:B:471[B]:ARG:HE	1:B:480:TYR:HE2	1.53	0.56
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.86	0.56
1:A:452[B]:GLU:HG3	8:A:877:HOH:O	2.06	0.55
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.05	0.55
1:B:535:ASP:HB3	1:B:538:LYS:HD2	1.89	0.54
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.89	0.54
1:B:50:LYS:HD3	8:B:1062:HOH:O	2.07	0.53
3:A:1150:NAG:H61	3:A:1151:NAG:H61	1.90	0.53
1:B:47:ASP:HA	1:B:52[B]:THR:HG23	1.91	0.52
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.44	0.52
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.45	0.51
3:B:2219:NAG:H82	8:B:1271:HOH:O	2.10	0.51
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TRP:CE2	1:A:212[B]:SER:HB2	2.47	0.49
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.94	0.49
1:A:154:TRP:CE2	1:A:212[A]:SER:HB3	2.49	0.48
1:B:69:LEU:HD11	1:B:107:ILE:CD1	2.37	0.48
3:A:1150:NAG:H4	3:A:1151:NAG:H2	1.59	0.47
1:A:78:VAL:HG23	1:A:89:PHE:HB2	1.96	0.47
1:A:40:ARG:HB2	1:A:506:ASN:O	2.14	0.47
1:A:55:LEU:HD12	1:A:500:LEU:CD2	2.45	0.47
1:B:513:LYS:O	1:B:527:GLN:HA	2.16	0.46
1:B:154:TRP:CE2	1:B:212[A]:SER:HB2	2.51	0.45
1:B:358:ARG:HD2	8:B:1061:HOH:O	2.17	0.45
1:B:501:ASP:O	1:B:505:GLN:HG2	2.18	0.43
1:A:726:VAL:HG23	1:A:728:VAL:HG23	2.00	0.43
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.43
1:A:170:ASN:N	1:A:170:ASN:HD22	2.16	0.43
1:B:696:LYS:CG	1:B:728:VAL:HG22	2.49	0.43
1:B:546:VAL:HG21	1:B:626:ILE:HD11	2.00	0.42
1:A:539:LYS:HE3	1:A:617:GLY:O	2.19	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.18	0.42
1:A:253[A]:ARG:HH21	1:B:253:ARG:HH21	1.67	0.42
1:A:453:ARG:HG3	1:A:476:GLY:HA3	2.02	0.42
1:A:709:ASP:O	1:A:712:HIS:HE1	2.02	0.41
1:B:345:HIS:HE1	1:B:389:ILE:O	2.02	0.41
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.55	0.41
1:B:154:TRP:CE2	1:B:212[B]:SER:HB3	2.56	0.41
1:B:60:LEU:HB2	1:B:68:TYR:CD1	2.56	0.41
1:A:53:TYR:HB3	1:A:500:LEU:HD11	2.01	0.41
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.34	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	738/728 (101%)	715 (97%)	23 (3%)	0	100	100
1	B	736/728 (101%)	715 (97%)	21 (3%)	0	100	100
All	All	1474/1456 (101%)	1430 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	665/653 (102%)	656 (99%)	9 (1%)	71	76
1	B	663/653 (102%)	653 (98%)	10 (2%)	70	74
All	All	1328/1306 (102%)	1309 (99%)	19 (1%)	71	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	116	LEU
1	A	170	ASN
1	A	230	ASP
1	A	263	ASN
1	A	366	LEU
1	A	385	CYS
1	A	472	CYS
1	A	627	TRP
1	B	51	ASN
1	B	97	GLU
1	B	230	ASP
1	B	272	ASN
1	B	385	CYS
1	B	450[A]	ASN
1	B	450[B]	ASN
1	B	472	CYS
1	B	487	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	685	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	263	ASN
1	A	388	GLN
1	A	435	GLN
1	A	572	ASN
1	A	694	ASN
1	A	712	HIS
1	B	74	ASN
1	B	75	ASN
1	B	169	ASN
1	B	272	ASN
1	B	345	HIS
1	B	487	ASN
1	B	533	HIS
1	B	572	ASN
1	B	685	ASN
1	B	694	ASN
1	B	712	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.59	0	15,19,21	2.08	4 (26%)
2	NDG	A	1086	2	14,14,15	0.53	0	15,19,21	1.21	2 (13%)
3	NAG	A	1150	1,3	14,14,15	0.57	0	15,19,21	1.08	1 (6%)
3	NAG	A	1151	3	14,14,15	0.67	1 (7%)	15,19,21	1.66	2 (13%)
3	NAG	A	1219	1,3	14,14,15	0.50	0	15,19,21	0.92	1 (6%)
3	NAG	A	1220	3	14,14,15	0.36	0	15,19,21	1.44	2 (13%)
2	NAG	A	1229	1,2	14,14,15	0.66	0	15,19,21	1.11	1 (6%)
2	NDG	A	1230	2	14,14,15	0.83	0	15,19,21	1.35	2 (13%)
3	NAG	A	1321	1,3	14,14,15	0.57	0	15,19,21	1.62	4 (26%)
3	NAG	A	1322	3	14,14,15	0.64	0	15,19,21	1.27	3 (20%)
3	NAG	B	2085	1,3	14,14,15	0.60	0	15,19,21	1.10	1 (6%)
3	NAG	B	2086	3	14,14,15	0.68	0	15,19,21	1.42	2 (13%)
3	NAG	B	2219	1,3	14,14,15	0.54	0	15,19,21	1.07	0
3	NAG	B	2220	3	14,14,15	0.60	0	15,19,21	1.51	2 (13%)
3	NAG	B	2229	1,3	14,14,15	0.61	0	15,19,21	1.13	1 (6%)
3	NAG	B	2230	3	14,14,15	0.54	0	15,19,21	0.90	0
3	NAG	B	2281	1,3	14,14,15	0.56	0	15,19,21	1.31	3 (20%)
3	NAG	B	2282	3	14,14,15	0.50	0	15,19,21	1.13	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
3	NAG	A	1150	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1151	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1219	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1220	3	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1321	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1322	3	-	2/6/23/26	0/1/1/1
3	NAG	B	2085	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2086	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2219	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2220	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2229	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2230	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2281	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2282	3	-	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)
3	A	1151	NAG	C1-C2	2.01	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1085	NAG	C4-C3-C2	-3.87	105.35	111.02
3	B	2229	NAG	O5-C1-C2	-3.32	106.86	111.47
3	A	1321	NAG	O4-C4-C3	-3.21	103.37	110.36
2	A	1086	NDG	O-C1-C2	-3.20	107.02	111.47
3	B	2281	NAG	O5-C1-C2	-3.00	107.30	111.47
3	A	1321	NAG	O5-C1-C2	-2.66	107.77	111.47
3	A	1220	NAG	C6-C5-C4	-2.24	107.75	113.00
3	A	1322	NAG	O5-C1-C2	-2.14	108.49	111.47
3	B	2281	NAG	C2-N2-C7	-2.04	119.97	122.94
2	A	1086	NDG	C3-C4-C5	2.02	113.78	110.22
3	A	1322	NAG	C4-C3-C2	2.16	114.18	111.02
3	A	1219	NAG	C1-O5-C5	2.24	115.25	112.17
2	A	1085	NAG	O5-C1-C2	2.28	114.64	111.47
3	A	1151	NAG	C2-N2-C7	2.49	126.58	122.94
3	B	2281	NAG	C1-O5-C5	2.51	115.62	112.17
2	A	1230	NDG	C2-N2-C7	2.52	126.63	122.94
3	A	1321	NAG	C4-C3-C2	2.53	114.72	111.02
3	B	2220	NAG	C3-C4-C5	2.56	114.73	110.22
3	A	1321	NAG	C1-O5-C5	2.78	116.00	112.17
2	A	1229	NAG	C1-O5-C5	2.79	116.02	112.17
3	A	1322	NAG	C3-C4-C5	2.80	115.15	110.22
3	B	2086	NAG	C3-C4-C5	2.99	115.48	110.22
3	B	2085	NAG	C4-C3-C2	3.09	115.55	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1150	NAG	C1-O5-C5	3.09	116.43	112.17
3	B	2282	NAG	C1-O5-C5	3.10	116.44	112.17
3	B	2086	NAG	C4-C3-C2	3.55	116.22	111.02
3	B	2220	NAG	C4-C3-C2	3.55	116.22	111.02
2	A	1230	NDG	C4-C3-C2	3.63	116.33	111.02
2	A	1085	NAG	C1-O5-C5	4.17	117.92	112.17
2	A	1085	NAG	O4-C4-C3	4.27	119.64	110.36
3	A	1220	NAG	C1-O5-C5	4.41	118.24	112.17
3	A	1151	NAG	C1-O5-C5	5.25	119.40	112.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1322	NAG	C8-C7-N2-C2
3	A	1322	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1150	NAG	2	0
3	A	1151	NAG	2	0
3	B	2219	NAG	1	0

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
4	NAG	A	1281	1	14,14,15	0.60	0	15,19,21	1.08	2 (13%)
6	361	A	767	-	22,26,26	1.50	4 (18%)	25,39,39	1.40	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	361	B	2	-	22,26,26	1.52	3 (13%)	25,39,39	1.58	6 (24%)
7	NDG	B	2092	1	14,14,15	0.53	0	15,19,21	1.20	1 (6%)
4	NAG	B	2150	1	14,14,15	0.50	0	15,19,21	1.13	1 (6%)
4	NAG	B	2321	1	14,14,15	0.55	0	15,19,21	1.39	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
4	NAG	A	1281	1	-	0/6/23/26	0/1/1/1
6	361	A	767	-	-	0/4/16/16	0/3/4/4
6	361	B	2	-	-	0/4/16/16	0/3/4/4
7	NDG	B	2092	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2150	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2321	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	767	361	C10-C11	2.02	1.52	1.50
6	A	767	361	C10-C9	2.51	1.55	1.53
6	B	2	361	C10-C11	2.59	1.53	1.50
6	A	767	361	C23-C22	3.18	1.40	1.36
6	B	2	361	C23-C22	3.33	1.41	1.36
6	B	2	361	C29-C19	3.48	1.47	1.40
6	A	767	361	C29-C19	3.92	1.48	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2	361	C11-C10-C9	-3.82	108.88	113.99
6	A	767	361	C11-C10-C9	-3.11	109.83	113.99
6	A	767	361	C20-C19-C29	-2.87	118.23	121.12
4	B	2321	NAG	O5-C1-C2	-2.44	108.08	111.47
6	B	2	361	C1-C2-C3	-2.41	120.51	123.66
6	B	2	361	C20-C19-C29	-2.21	118.90	121.12
6	A	767	361	C23-C22-N21	-2.04	121.01	123.73
4	A	1281	NAG	O5-C1-C2	-2.04	108.64	111.47
6	B	2	361	C3-C9-C14	-2.00	108.34	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	767	361	C4-C3-C2	2.38	119.05	116.15
6	B	2	361	C4-C3-C2	2.41	119.08	116.15
6	B	2	361	C22-N21-C20	2.49	123.21	117.27
6	A	767	361	C22-N21-C20	2.60	123.46	117.27
4	A	1281	NAG	C1-O5-C5	2.66	115.83	112.17
4	B	2150	NAG	C1-O5-C5	3.25	116.65	112.17
4	B	2321	NAG	C1-O5-C5	4.01	117.69	112.17
7	B	2092	NDG	C1-O-C5	4.19	117.94	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	728/728 (100%)	0.15	23 (3%)	48	48	25, 33, 46, 59	0
1	B	728/728 (100%)	0.18	27 (3%)	42	43	26, 33, 46, 62	0
All	All	1456/1456 (100%)	0.17	50 (3%)	46	46	25, 33, 47, 62	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	THR	6.1
1	A	39	THR	5.8
1	B	766	PRO	5.3
1	B	73	GLU	4.7
1	A	74	ASN	4.6
1	A	279	VAL	3.9
1	A	97	GLU	3.9
1	A	73	GLU	3.7
1	B	40	ARG	3.6
1	B	96	ASP	3.6
1	A	766	PRO	3.6
1	B	333	SER	3.5
1	B	92	ASN	3.4
1	B	97	GLU	3.2
1	B	378	GLU	3.2
1	B	74	ASN	3.1
1	B	334	SER	3.0
1	A	92	ASN	3.0
1	A	93	SER	2.9
1	A	40	ARG	2.8
1	B	529	ILE	2.8
1	A	41	LYS	2.7
1	A	138	ASN	2.7
1	A	506	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	521	GLU	2.6
1	B	99	GLY	2.5
1	B	506	ASN	2.5
1	B	765	LEU	2.5
1	B	91	GLU	2.5
1	A	546[A]	VAL	2.5
1	B	332	GLU	2.4
1	A	166	TYR	2.4
1	A	75	ASN	2.4
1	A	333	SER	2.4
1	A	332	GLU	2.3
1	B	88	VAL	2.3
1	A	164	LEU	2.3
1	B	313	LEU	2.3
1	B	575	VAL	2.2
1	B	138	ASN	2.2
1	A	96	ASP	2.2
1	A	98	PHE	2.1
1	A	140	ARG	2.1
1	B	100	HIS	2.1
1	B	300	LEU	2.1
1	B	502	LYS	2.0
1	B	172	ILE	2.0
1	B	519	LEU	2.0
1	A	99	GLY	2.0
1	B	140	ARG	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, 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(\AA^2)	Q<0.9
3	NAG	A	1219	14/15	0.89	0.26	10.78	45,49,53,54	0
3	NAG	A	1321	14/15	0.81	0.29	6.08	49,53,56,61	0
3	NAG	B	2219	14/15	0.92	0.26	4.67	36,42,47,49	0
2	NAG	A	1085	14/15	0.81	0.26	4.61	52,56,62,66	0
3	NAG	B	2085	14/15	0.85	0.17	3.34	52,58,64,69	0
3	NAG	A	1220	14/15	0.80	0.33	2.08	56,58,61,63	0
3	NAG	B	2220	14/15	0.87	0.31	2.07	47,51,55,56	0
2	NAG	A	1229	14/15	0.94	0.18	1.17	39,44,48,54	0
3	NAG	B	2229	14/15	0.94	0.18	1.09	32,34,41,44	0
3	NAG	B	2281	14/15	0.92	0.10	-1.68	37,40,46,51	0
2	NDG	A	1230	14/15	0.74	0.38	-	60,63,68,69	0
3	NAG	A	1150	14/15	0.80	0.41	-	57,61,65,70	0
2	NDG	A	1086	14/15	0.54	0.46	-	70,73,74,74	0
3	NAG	B	2230	14/15	0.83	0.38	-	48,52,54,55	0
3	NAG	A	1151	14/15	0.54	0.51	-	73,75,77,77	0
3	NAG	B	2282	14/15	0.68	0.26	-	55,59,60,60	0
3	NAG	A	1322	14/15	0.62	0.46	-	66,68,70,70	0
3	NAG	B	2086	14/15	0.42	0.38	-	73,76,77,77	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(\AA^2)	Q<0.9
4	NAG	B	2321	14/15	0.76	0.32	5.90	45,49,51,52	0
5	NA	A	1	1/1	0.97	0.12	-0.72	31,31,31,31	0
6	361	A	767	23/23	0.96	0.09	-1.21	28,34,35,35	0
6	361	B	2	23/23	0.96	0.09	-1.28	30,34,36,36	0
4	NAG	A	1281	14/15	0.81	0.25	-	51,55,57,57	0
7	NDG	B	2092	14/15	0.69	0.48	-	71,74,76,76	0
4	NAG	B	2150	14/15	0.77	0.40	-	56,60,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.