



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 PM UTC

PDB ID : 1DMT / pdb_00001dmt
Title : STRUCTURE OF HUMAN NEUTRAL ENDOPEPTIDASE COMPLEXED
WITH PHOSPHORAMIDON
Authors : Oefner, C.; D'Arcy, A.; Hennig, M.; Winkler, F.K.; Dale, G.E.
Deposited on : 1999-12-15
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

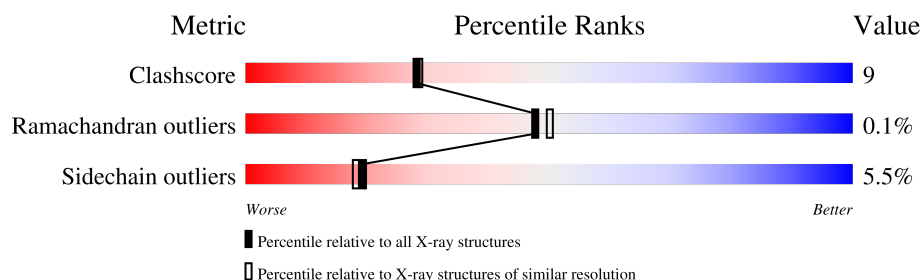
1 Overall quality at a glance

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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	696	 81% 16% .

2 Entry composition [i](#)

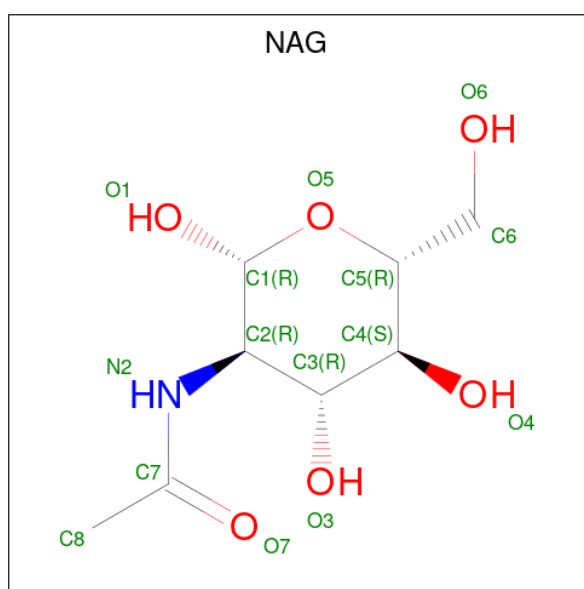
There are 6 unique types of molecules in this entry. The entry contains 6146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEUTRAL ENDOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	696	5595	3538	957	1074	26	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

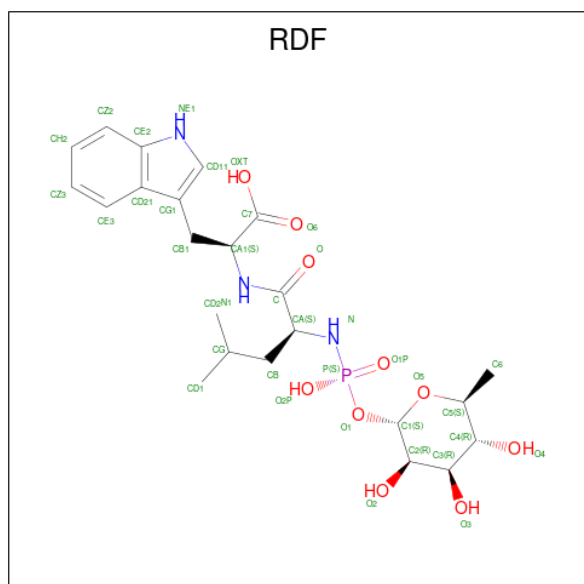


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

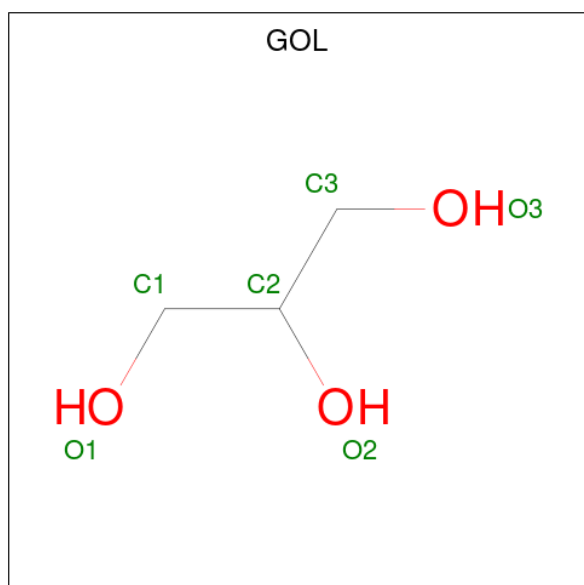
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is N-ALPHA-L-RHAMNOPYRANOSYLOXY(HYDROXYPHOSPHINYL)-L-L EUCYL-L-TRYPTOPHAN (CCD ID: RDF) (formula: $C_{23}H_{34}N_3O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			37	23	3	10	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	465	Total	O	0	0
			465	465		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

• Molecule 1: NEUTRAL ENDOPEPTIDASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.58Å 107.58Å 112.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.4 (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6146	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, GOL, RDF

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	0.55	2/5713 (0.0%)	0.97	17/7727 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	460	MET	SD-CE	-5.66	1.65	1.79
1	A	370	MET	SD-CE	-5.62	1.65	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	SER	N-CA-C	-8.96	98.70	110.53
1	A	232	GLU	N-CA-C	-8.80	101.77	111.36
1	A	168	VAL	CB-CA-C	-7.45	101.18	112.05
1	A	391	ASN	N-CA-C	7.04	119.60	111.02
1	A	430	ALA	N-CA-C	6.46	123.30	113.61
1	A	318	LYS	CA-C-N	6.45	142.47	127.00
1	A	318	LYS	C-N-CA	6.45	142.47	127.00
1	A	717	ARG	N-CA-C	-6.13	104.68	111.36
1	A	192	SER	N-CA-C	5.91	119.67	112.23
1	A	479	ILE	N-CA-C	5.49	115.76	107.75
1	A	681	HIS	N-CA-C	5.47	118.17	111.82
1	A	318	LYS	C-N-CD	-5.42	108.69	120.60
1	A	705	SER	N-CA-C	5.23	117.72	111.71
1	A	607	THR	N-CA-C	-5.14	103.61	110.55
1	A	318	LYS	N-CA-C	5.13	121.15	109.81
1	A	225	LEU	CA-C-N	5.05	124.49	119.24
1	A	225	LEU	C-N-CA	5.05	124.49	119.24

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	5595	0	5447	93	0
2	A	42	0	39	0	0
3	A	1	0	0	0	0
4	A	37	0	32	7	0
5	A	6	0	8	0	0
6	A	465	0	0	2	0
All	All	6146	0	5526	100	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.

All (100) 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)
4:A:750:RDF:CD21	4:A:750:RDF:CG1	1.44	1.14
4:A:750:RDF:HD1	4:A:750:RDF:CD11	0.97	1.07
4:A:750:RDF:CG1	4:A:750:RDF:NE1	2.25	0.96
4:A:750:RDF:CG1	4:A:750:RDF:HD1	2.08	0.82
1:A:636:GLN:HE22	1:A:707:LYS:NZ	1.84	0.76
1:A:333:VAL:CG1	1:A:523:LYS:HG2	2.15	0.76
4:A:750:RDF:CG1	4:A:750:RDF:CE3	2.64	0.75
1:A:168:VAL:H	1:A:368:ASN:HD21	1.35	0.74
1:A:318:LYS:HB3	1:A:319:PRO:C	2.13	0.73
1:A:440:GLU:HG3	1:A:479:ILE:HD12	1.73	0.70
1:A:354:LEU:HG	1:A:358:LEU:HD22	1.73	0.70
4:A:750:RDF:CE3	4:A:750:RDF:CE2	2.46	0.68
4:A:750:RDF:HD1	4:A:750:RDF:NE1	2.10	0.66
1:A:301:LYS:HD2	1:A:342:ASP:HB3	1.79	0.64
1:A:333:VAL:HG11	1:A:523:LYS:HG2	1.78	0.64
1:A:333:VAL:HG13	1:A:523:LYS:HG2	1.78	0.63
1:A:636:GLN:HE22	1:A:707:LYS:HZ3	1.45	0.63
1:A:182:THR:HG23	1:A:184:GLU:HG2	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:OG1	1:A:306:GLN:HG3	1.99	0.62
1:A:333:VAL:HG12	1:A:333:VAL:O	2.01	0.61
1:A:168:VAL:HG22	1:A:368:ASN:ND2	2.16	0.60
1:A:189:GLN:OE1	1:A:193:LYS:HE3	2.01	0.60
1:A:272:MET:O	1:A:275:VAL:HG22	2.03	0.59
1:A:355:LYS:HB3	1:A:356:PRO:HD3	1.86	0.58
1:A:597:ASN:ND2	1:A:601:ASP:H	2.03	0.57
1:A:597:ASN:HD22	1:A:597:ASN:C	2.10	0.57
1:A:507:PHE:CE1	1:A:511:ILE:HD11	2.40	0.57
1:A:101:SER:OG	1:A:398:TYR:HB3	2.03	0.57
1:A:704:ASN:HD22	1:A:704:ASN:C	2.13	0.57
1:A:253:ARG:HG3	1:A:263:ILE:HD13	1.87	0.56
1:A:502:LYS:H	1:A:509:ASN:HD21	1.53	0.56
1:A:159:LEU:HD22	1:A:511:ILE:HD11	1.87	0.56
1:A:156:LEU:HD22	1:A:160:LEU:HD13	1.88	0.56
1:A:67:ARG:HH22	1:A:688:ASN:HD21	1.52	0.55
1:A:636:GLN:NE2	1:A:707:LYS:NZ	2.53	0.55
1:A:67:ARG:HH12	1:A:688:ASN:ND2	2.04	0.55
1:A:182:THR:HG22	1:A:185:LYS:HB2	1.89	0.54
1:A:67:ARG:HH22	1:A:688:ASN:ND2	2.07	0.53
1:A:54:GLY:O	1:A:673:LEU:HD12	2.08	0.53
1:A:338:THR:HG22	1:A:339:ASN:H	1.74	0.52
1:A:218:ILE:HD13	1:A:322:TRP:CZ3	2.45	0.51
1:A:182:THR:CG2	1:A:184:GLU:HG2	2.41	0.51
1:A:353:LYS:O	1:A:356:PRO:HD2	2.11	0.51
1:A:691:GLN:HA	1:A:694:CYS:SG	2.50	0.51
1:A:57:LYS:HD2	1:A:57:LYS:H	1.77	0.50
1:A:202:LEU:HD13	1:A:216:ILE:HG23	1.93	0.50
1:A:167:PRO:HB2	1:A:368:ASN:ND2	2.28	0.49
1:A:184:GLU:HG3	1:A:324:ASN:OD1	2.12	0.49
1:A:318:LYS:HB3	1:A:319:PRO:CA	2.43	0.48
1:A:440:GLU:HG3	1:A:479:ILE:CD1	2.43	0.48
1:A:336:SER:C	1:A:337:ILE:HD12	2.39	0.48
1:A:394:ARG:HH21	1:A:402:SER:N	2.11	0.48
1:A:78:PRO:HG3	1:A:85:TYR:CE1	2.49	0.48
1:A:168:VAL:HG11	1:A:272:MET:HE3	1.97	0.47
1:A:202:LEU:CD1	1:A:216:ILE:HG23	2.44	0.47
1:A:476:LYS:HE2	1:A:478:ARG:NH1	2.29	0.47
1:A:68:LEU:HD22	1:A:687:LEU:HD13	1.96	0.47
1:A:182:THR:CG2	1:A:185:LYS:H	2.28	0.46
1:A:304:LEU:HD23	1:A:307:ILE:HD12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:HG23	1:A:185:LYS:H	1.80	0.46
1:A:248:MET:SD	1:A:275:VAL:CG2	3.04	0.46
1:A:248:MET:HB3	1:A:272:MET:SD	2.55	0.46
1:A:542:ASN:O	1:A:555:PRO:HD2	2.16	0.46
1:A:102:ARG:HD3	1:A:697:TYR:CE1	2.51	0.46
1:A:727:GLU:H	1:A:727:GLU:CD	2.24	0.45
1:A:636:GLN:HE22	1:A:707:LYS:HZ1	1.64	0.45
1:A:589:PHE:HB3	1:A:749:TRP:CZ2	2.52	0.45
1:A:55:ILE:O	1:A:57:LYS:HE3	2.17	0.45
1:A:338:THR:HG22	1:A:339:ASN:N	2.32	0.44
1:A:67:ARG:HH12	1:A:688:ASN:HD22	1.65	0.44
1:A:394:ARG:HH21	1:A:401:THR:C	2.26	0.44
1:A:333:VAL:HG11	1:A:523:LYS:HA	1.99	0.44
1:A:597:ASN:HD21	1:A:601:ASP:H	1.65	0.44
1:A:78:PRO:HG3	1:A:85:TYR:CD1	2.53	0.44
1:A:253:ARG:O	1:A:257:GLN:HG3	2.17	0.44
1:A:167:PRO:HB3	1:A:364:ARG:HG3	2.00	0.44
1:A:257:GLN:NE2	6:A:957:HOH:O	2.50	0.43
1:A:333:VAL:CG1	1:A:333:VAL:O	2.66	0.43
1:A:120:VAL:O	1:A:136:LYS:HE2	2.18	0.43
1:A:424:ARG:HD2	1:A:485:ILE:O	2.19	0.43
1:A:347:ALA:HB1	1:A:350:TYR:HB3	2.01	0.43
1:A:272:MET:HA	1:A:272:MET:HE2	2.00	0.42
1:A:81:ASP:OD2	1:A:84:LYS:HD3	2.20	0.42
1:A:163:ILE:O	1:A:164:TYR:HB2	2.19	0.42
1:A:248:MET:HG2	1:A:372:TRP:CE2	2.55	0.42
1:A:102:ARG:HD3	1:A:697:TYR:CZ	2.54	0.42
1:A:673:LEU:HD12	1:A:673:LEU:H	1.85	0.42
1:A:476:LYS:O	1:A:551:GLN:HB2	2.18	0.42
1:A:295:PRO:HG3	1:A:592:ASN:ND2	2.35	0.41
1:A:478:ARG:NH2	1:A:532:ASP:HA	2.35	0.41
1:A:168:VAL:N	1:A:368:ASN:HD21	2.11	0.41
1:A:604:ASP:HA	6:A:1007:HOH:O	2.20	0.41
1:A:478:ARG:HH22	1:A:532:ASP:HA	1.86	0.41
1:A:533:GLU:HB3	1:A:549:ARG:HH12	1.86	0.41
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.95	0.41
1:A:278:LEU:HD11	1:A:366:LEU:HD23	2.03	0.41
1:A:643:THR:HA	1:A:710:VAL:O	2.20	0.41
1:A:368:ASN:HD22	1:A:368:ASN:HA	1.66	0.41
1:A:298:LEU:HD22	1:A:346:TYR:O	2.20	0.40
1:A:123:GLU:HA	1:A:124:PRO:HD3	1.95	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	694/696 (100%)	676 (97%)	17 (2%)	1 (0%)	48 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	LYS

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	605/605 (100%)	572 (94%)	33 (6%)	19 18

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	77	GLU
1	A	91	LEU
1	A	101	SER
1	A	156	LEU
1	A	160	LEU
1	A	168	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	182	THR
1	A	184	GLU
1	A	196	LYS
1	A	202	LEU
1	A	215	VAL
1	A	260	ARG
1	A	266	ASN
1	A	278	LEU
1	A	298	LEU
1	A	318	LYS
1	A	358	LEU
1	A	368	ASN
1	A	379	VAL
1	A	414	VAL
1	A	477	GLU
1	A	490	ASN
1	A	492	LEU
1	A	497	LEU
1	A	498	GLU
1	A	597	ASN
1	A	602	LEU
1	A	673	LEU
1	A	687	LEU
1	A	692	VAL
1	A	704	ASN
1	A	748	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	267	GLN
1	A	306	GLN
1	A	368	ASN
1	A	490	ASN
1	A	509	ASN
1	A	550	ASN
1	A	592	ASN
1	A	597	ASN
1	A	608	GLN
1	A	619	GLN
1	A	636	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	637	HIS
1	A	656	GLN
1	A	662	GLN
1	A	688	ASN
1	A	704	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
2	NAG	A	753	1	14,14,15	0.46	0	17,19,21	0.56	0
2	NAG	A	754	1	14,14,15	0.36	0	17,19,21	0.75	1 (5%)
5	GOL	A	751	-	5,5,5	1.01	0	5,5,5	1.24	0
4	RDF	A	750	3	38,39,39	2.12	9 (23%)	53,57,57	1.42	7 (13%)
2	NAG	A	752	1	14,14,15	0.43	0	17,19,21	0.73	0

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	753	1	-	1/6/23/26	0/1/1/1
2	NAG	A	754	1	-	2/6/23/26	0/1/1/1
5	GOL	A	751	-	-	1/4/4/4	-
4	RDF	A	750	3	-	1/27/50/50	0/3/3/3
2	NAG	A	752	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	750	RDF	P-N	6.42	1.69	1.61
4	A	750	RDF	C-N1	5.79	1.46	1.34
4	A	750	RDF	P-O2P	-4.15	1.45	1.56
4	A	750	RDF	CH2-CZ3	3.66	1.46	1.38
4	A	750	RDF	CA-N	3.47	1.51	1.47
4	A	750	RDF	CE3-CD21	2.76	1.44	1.39
4	A	750	RDF	P-O1P	2.70	1.50	1.46
4	A	750	RDF	CZ2-CE2	2.44	1.43	1.39
4	A	750	RDF	OXT-C7	-2.31	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	750	RDF	O1P-P-N	-4.00	106.42	112.75
4	A	750	RDF	CA1-N1-C	-3.22	114.72	121.65
4	A	750	RDF	O2P-P-O1P	3.21	116.76	109.87
4	A	750	RDF	O-C-CA	3.21	127.20	120.48
4	A	750	RDF	O1-P-O1P	-3.02	110.05	115.32
4	A	750	RDF	O-C-N1	-3.00	117.59	122.96
4	A	750	RDF	CA1-CB1-CG1	-2.18	109.32	113.44
2	A	754	NAG	C2-N2-C7	-2.08	120.12	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	754	NAG	C4-C5-C6-O6
2	A	754	NAG	O5-C5-C6-O6
5	A	751	GOL	C1-C2-C3-O3
2	A	753	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

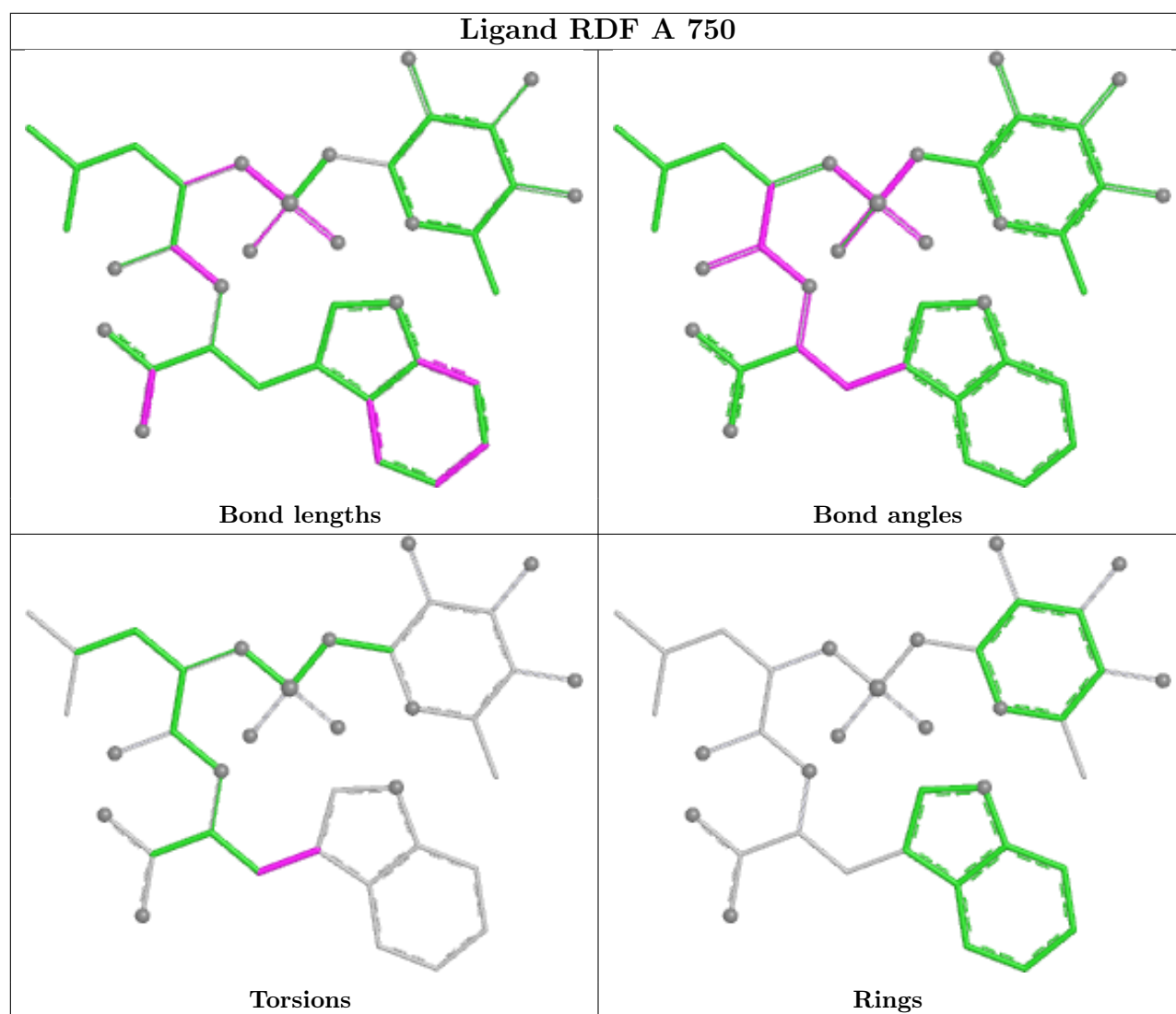
Mol	Chain	Res	Type	Atoms
4	A	750	RDF	CA1-CB1-CG1-CD21

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	750	RDF	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.