



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:22 PM BST

PDB ID : 1K3B
Title : Crystal Structure of Human Dipeptidyl Peptidase I (Cathepsin C): Exclusion Domain Added to an Endopeptidase Framework Creates the Machine for Activation of Granular Serine Proteases
Authors : Turk, D.; Janjic, V.; Stern, I.; Podobnik, M.; Lamba, D.; Dahl, S.W.; Lauritzen, C.; Pedersen, J.; Turk, V.; Turk, B.
Deposited on : 2001-10-02
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

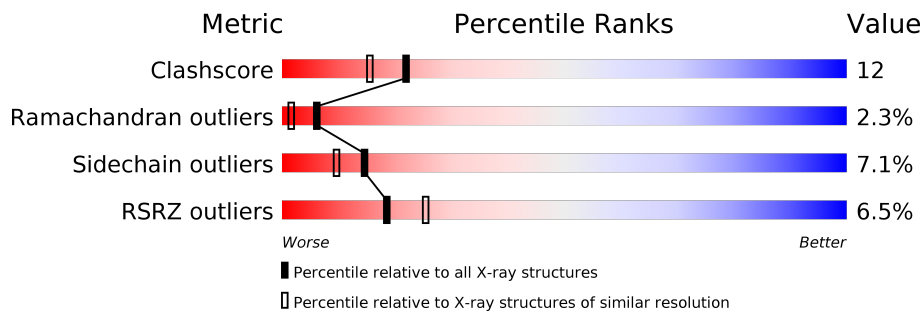
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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 $\leq 5\%$. 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	119	 8% 75% 17% 8%
2	B	164	 5% 76% 20% ..
3	C	69	 7% 77% 23%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3278 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 I exclusion domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	119	950	610	154	180	6	27	0	0

- Molecule 2 is a protein called dipeptidyl-peptidase I light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	164	1298	828	216	241	13	14	0	0

- Molecule 3 is a protein called dipeptidyl-peptidase I heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	69	536	343	89	102	2	8	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
5	B	1	5	4	1	0	0
5	C	1	5	4	1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	B	1	1	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	152	152	152	0	0
7	B	246	246	246	0	0

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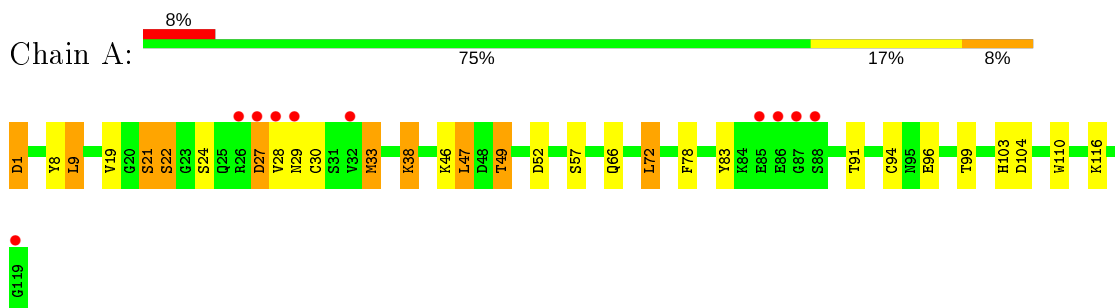
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	66	Total	O	0	0
			66	66		

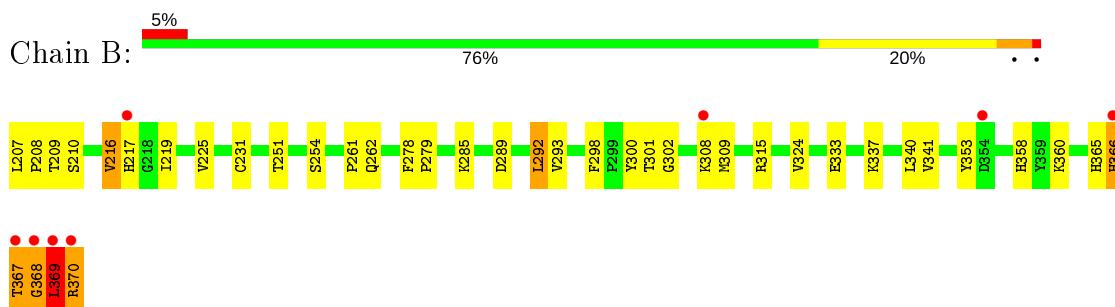
3 Residue-property plots [i](#)

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 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.

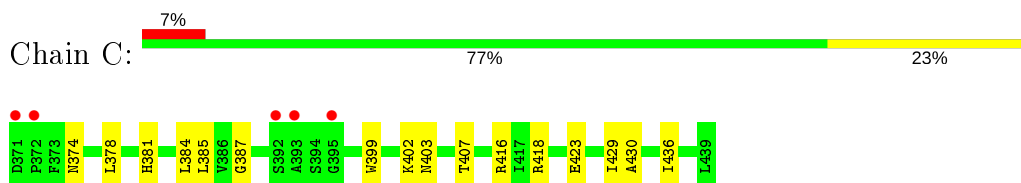
- Molecule 1: dipeptidyl-peptidase I exclusion domain



- Molecule 2: dipeptidyl-peptidase I light chain



- Molecule 3: dipeptidyl-peptidase I heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.15Å 88.03Å 114.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.15 20.64 – 2.15	Depositor EDS
% Data completeness (in resolution range)	5.0 (10.00-2.15) 97.1 (20.64-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.15Å)	Xtrriage
Refinement program	MAIN	Depositor
R, R_{free}	0.190 , 0.231 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtrriage
Anisotropy	0.313	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3278	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, 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	0.45	0/975	0.81	1/1322 (0.1%)
2	B	0.45	0/1338	0.71	2/1811 (0.1%)
3	C	0.43	0/552	0.68	0/752
All	All	0.45	0/2865	0.74	3/3885 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	368	GLY	N-CA-C	6.93	130.44	113.10
1	A	72	LEU	CA-CB-CG	5.91	128.89	115.30
2	B	366	HIS	N-CA-C	5.65	126.26	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	950	0	901	26	0
2	B	1298	0	1207	36	0
3	C	536	0	505	13	1
4	A	14	0	13	2	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	B	1	0	0	0	0
7	A	152	0	0	7	1
7	B	246	0	0	6	1
7	C	66	0	0	0	0
All	All	3278	0	2626	63	2

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 12.

All (63) 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:9:LEU:HD12	3:C:374:ASN:ND2	1.39	1.37
1:A:9:LEU:CD1	3:C:374:ASN:HD21	1.66	1.08
1:A:9:LEU:CD1	3:C:374:ASN:ND2	2.26	0.96
1:A:9:LEU:HD12	3:C:374:ASN:HD21	0.92	0.92
2:B:367:THR:HG22	2:B:368:GLY:H	1.38	0.87
1:A:29:ASN:HB3	7:A:1069:HOH:O	1.86	0.75
1:A:49:THR:HG22	7:A:1379:HOH:O	1.85	0.75
1:A:24:SER:H	1:A:27:ASP:HB2	1.55	0.71
2:B:370:ARG:HA	7:B:1240:HOH:O	1.88	0.71
1:A:103:HIS:HD2	1:A:104:ASP:O	1.78	0.67
2:B:365:HIS:CE1	2:B:366:HIS:HB3	2.32	0.64
1:A:30:CYS:HB3	1:A:99:THR:HG22	1.81	0.63
1:A:19:VAL:HB	1:A:38:LYS:HG2	1.80	0.62
1:A:94:CYS:HB2	7:A:1026:HOH:O	2.01	0.60
2:B:368:GLY:O	2:B:369:LEU:HB2	2.02	0.59
2:B:367:THR:HG22	2:B:368:GLY:N	2.16	0.56
3:C:381:HIS:HE1	3:C:403:ASN:OD1	1.88	0.55
1:A:78:PHE:HB3	2:B:285:LYS:HE2	1.89	0.55
2:B:370:ARG:HG3	7:B:1348:HOH:O	2.08	0.54
4:A:504:NAG:H3	3:C:378:LEU:HD13	1.89	0.54
1:A:30:CYS:HA	7:A:1444:HOH:O	2.07	0.53
1:A:78:PHE:CB	2:B:285:LYS:HE2	2.38	0.53
2:B:353:TYR:HB3	2:B:367:THR:HG21	1.90	0.53
2:B:365:HIS:HD2	3:C:423:GLU:OE2	1.92	0.52
1:A:52:ASP:HB2	7:A:1024:HOH:O	2.09	0.51
2:B:353:TYR:CD2	2:B:367:THR:HB	2.44	0.51
2:B:261:PRO:HD2	7:B:1099:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:TYR:CZ	2:B:368:GLY:HA3	2.45	0.51
2:B:231:CYS:HB2	2:B:302:GLY:O	2.10	0.50
2:B:292:LEU:O	2:B:315:ARG:HA	2.12	0.50
2:B:225:VAL:HB	3:C:407:THR:HG22	1.93	0.49
2:B:262:GLN:HB2	2:B:300:TYR:HA	1.94	0.49
2:B:207:LEU:N	7:B:1383:HOH:O	2.47	0.48
1:A:21:SER:O	1:A:22:SER:HB2	2.14	0.48
2:B:293:VAL:HG21	2:B:309:MET:HE3	1.96	0.48
1:A:83:TYR:HA	1:A:91:THR:O	2.14	0.47
2:B:337:LYS:O	2:B:341:VAL:HG13	2.14	0.47
2:B:293:VAL:HG12	2:B:315:ARG:HG2	1.96	0.46
1:A:96:GLU:HG2	1:A:116:LYS:HG2	1.99	0.45
2:B:219:ILE:HD12	7:B:1105:HOH:O	2.15	0.45
1:A:33:MET:N	7:A:1444:HOH:O	2.46	0.45
2:B:216:VAL:O	2:B:216:VAL:HG22	2.16	0.44
2:B:333:GLU:OE1	2:B:337:LYS:NZ	2.49	0.44
1:A:21:SER:O	1:A:22:SER:CB	2.65	0.43
3:C:399:TRP:O	3:C:416:ARG:HA	2.19	0.43
1:A:22:SER:HA	1:A:110:TRP:O	2.18	0.43
4:A:504:NAG:H83	7:A:1025:HOH:O	2.19	0.43
2:B:340:LEU:HD21	3:C:387:GLY:HA2	2.01	0.42
2:B:293:VAL:HG21	2:B:309:MET:CE	2.48	0.42
1:A:1:ASP:HA	1:A:66:GLN:OE1	2.20	0.42
3:C:385:LEU:HD11	3:C:399:TRP:CE3	2.55	0.42
2:B:217:HIS:HB2	7:B:1136:HOH:O	2.18	0.42
2:B:278:PHE:HA	2:B:279:PRO:HD3	1.92	0.42
1:A:103:HIS:HE1	2:B:289:ASP:OD1	2.03	0.42
1:A:66:GLN:HG3	2:B:278:PHE:CE1	2.55	0.41
2:B:353:TYR:CG	2:B:367:THR:HB	2.56	0.41
2:B:293:VAL:HG11	2:B:309:MET:CE	2.51	0.41
1:A:8:TYR:OH	1:A:47:LEU:N	2.54	0.41
2:B:207:LEU:HA	2:B:208:PRO:HD3	1.82	0.41
2:B:225:VAL:HA	3:C:402:LYS:HE2	2.03	0.40
1:A:24:SER:N	1:A:27:ASP:HB2	2.31	0.40
2:B:324:VAL:HG13	3:C:430:ALA:HB3	2.03	0.40
2:B:251:THR:O	2:B:254:SER:HB2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1295:HOH:O	7:B:1295:HOH:O[4_555]	2.06	0.14
3:C:436:ILE:CD1	7:A:1431:HOH:O[2_655]	2.15	0.05

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	117/119 (98%)	103 (88%)	9 (8%)	5 (4%)	2	0
2	B	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	7
3	C	67/69 (97%)	63 (94%)	3 (4%)	1 (2%)	10	5
All	All	346/352 (98%)	318 (92%)	20 (6%)	8 (2%)	6	1

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	22	SER
1	A	33	MET
2	B	367	THR
2	B	369	LEU
1	A	46	LYS
1	A	47	LEU
3	C	429	ILE

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	103/103 (100%)	95 (92%)	8 (8%)	12	7
2	B	138/138 (100%)	127 (92%)	11 (8%)	12	7
3	C	55/55 (100%)	53 (96%)	2 (4%)	35	33
All	All	296/296 (100%)	275 (93%)	21 (7%)	14	9

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	9	LEU
1	A	27	ASP
1	A	28	VAL
1	A	38	LYS
1	A	49	THR
1	A	57	SER
1	A	72	LEU
2	B	209	THR
2	B	210	SER
2	B	216	VAL
2	B	292	LEU
2	B	298	PHE
2	B	301	THR
2	B	308	LYS
2	B	358	HIS
2	B	360	LYS
2	B	369	LEU
2	B	370	ARG
3	C	384	LEU
3	C	418	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	56	ASN
1	A	103	HIS
2	B	228	GLN
2	B	365	HIS
3	C	374	ASN
3	C	381	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
5	SO4	B	502	-	4,4,4	0.19	0	6,6,6	0.24	0
4	NAG	A	504	1	14,14,15	0.60	0	17,19,21	0.99	2 (11%)
5	SO4	A	503	-	4,4,4	0.76	0	6,6,6	0.48	0
5	SO4	C	501	-	4,4,4	0.53	0	6,6,6	0.21	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
4	NAG	A	504	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	504	NAG	C4-C3-C2	2.22	114.28	111.02
4	A	504	NAG	C2-N2-C7	-2.17	119.81	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	NAG	O5-C5-C6-O6
4	A	504	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	NAG	2	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, 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	119/119 (100%)	0.05	10 (8%) 11 15	8, 16, 57, 61	9 (7%)
2	B	164/164 (100%)	-0.17	8 (4%) 29 38	7, 15, 39, 65	4 (2%)
3	C	69/69 (100%)	-0.11	5 (7%) 15 21	8, 16, 49, 60	2 (2%)
All	All	352/352 (100%)	-0.08	23 (6%) 18 25	7, 16, 49, 65	15 (4%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	368	GLY	10.5
2	B	367	THR	7.3
2	B	369	LEU	6.1
3	C	392	SER	4.3
1	A	29	ASN	4.0
1	A	27	ASP	4.0
1	A	88	SER	3.8
1	A	28	VAL	3.7
1	A	86	GLU	3.6
1	A	26	ARG	3.5
1	A	119	GLY	3.5
3	C	372	PRO	3.5
1	A	87	GLY	3.5
3	C	371	ASP	3.4
3	C	393	ALA	3.2
1	A	32	VAL	3.1
2	B	370	ARG	2.9
2	B	366	HIS	2.4
2	B	354	ASP	2.3
3	C	395	GLY	2.3
2	B	217	HIS	2.2
2	B	308	LYS	2.2
1	A	85	GLU	2.1

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](#)

There are no monosaccharides in this entry.

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. 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	B-factors(\AA^2)	Q<0.9
4	NAG	A	504	14/15	0.78	0.24	41,45,53,54	0
5	SO4	A	503	5/5	0.80	0.22	58,59,62,62	0
5	SO4	B	502	5/5	0.94	0.12	60,61,63,63	0
5	SO4	C	501	5/5	0.94	0.12	48,51,51,53	0
6	CL	B	500	1/1	0.99	0.03	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.