



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:46 PM GMT

PDB ID : 1LYB  
Title : CRYSTAL STRUCTURES OF NATIVE AND INHIBITED FORMS OF HUMAN CATHEPSIN D: IMPLICATIONS FOR LYSOSOMAL TARGETING AND DRUG DESIGN  
Authors : Baldwin, E.T.; Bhat, T.N.; Gulnik, S.; Erickson, J.W.  
Deposited on : 1993-04-22  
Resolution : 2.50 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

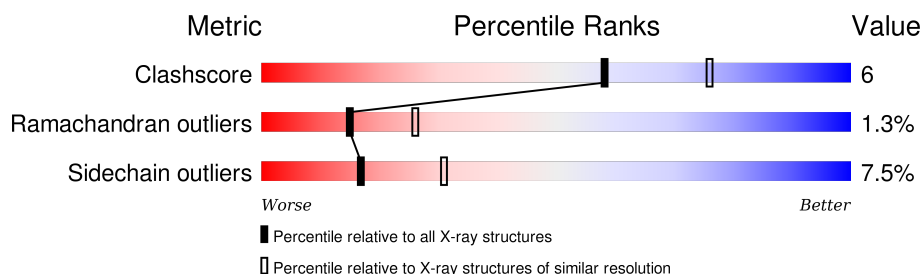
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	97	<div> <div>71%</div> <div>27%</div> <div>.</div> </div>
1	C	97	<div> <div>81%</div> <div>19%</div> </div>
2	B	241	<div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	D	241	<div> <div>73%</div> <div>24%</div> <div>.</div> </div>
3	I	6	<div> <div>33%</div> <div>50%</div> <div>17%</div> </div>
3	J	6	<div> <div>33%</div> <div>50%</div> <div>17%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6766 atoms, of which 1312 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 CATHEPSIN D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	97	Total	C	H	N	O	S	0	0	0
			904	478	156	119	146	5			
1	C	97	Total	C	H	N	O	S	0	0	0
			904	478	156	119	146	5			

- Molecule 2 is a protein called CATHEPSIN D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	241	Total	C	H	N	O	S	0	0	0
			2234	1184	389	302	348	11			
2	D	241	Total	C	H	N	O	S	0	0	0
			2234	1184	389	302	348	11			

- Molecule 3 is a protein called PEPSTATIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	6	Total	C	H	N	O	0	0	0
			55	34	7	5	9			
3	J	6	Total	C	H	N	O	0	0	0
			55	34	7	5	9			

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	4	Total	C	H	N	O	0	0
			96	28	46	2	20		
4	C	4	Total	C	H	N	O	0	0
			96	28	46	2	20		

- Molecule 5 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
5	B	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	D	1	Total 28	C 8	H 14	N 1	O 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	9	Total	H	O	0	0
			27	18	9		
6	B	13	Total	H	O	0	0
			39	26	13		
6	C	9	Total	H	O	0	0
			27	18	9		
6	D	13	Total	H	O	0	0
			39	26	13		

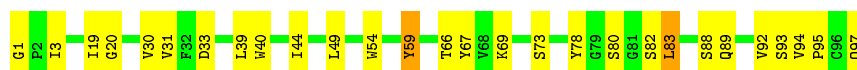
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.


Note EDS was not executed.

#### • Molecule 1: CATHEPSIN D

Chain A: 



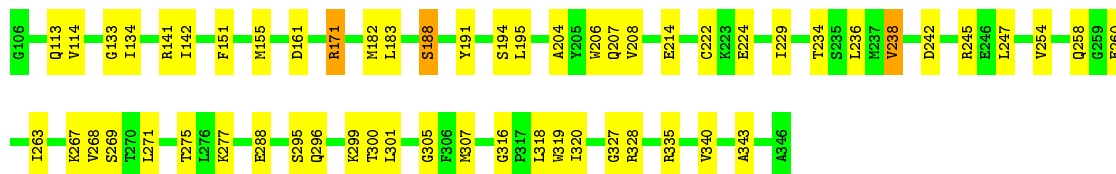
#### • Molecule 1: CATHEPSIN D

Chain C: 



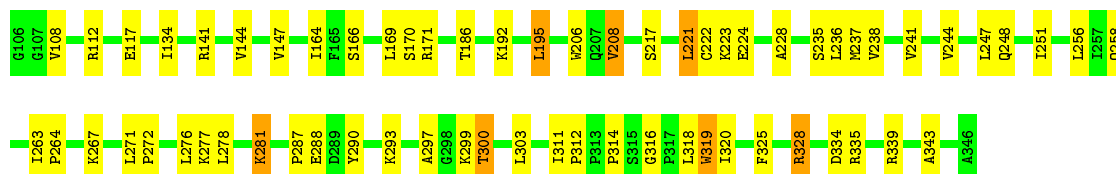
#### • Molecule 2: CATHEPSIN D

Chain B: 



#### • Molecule 2: CATHEPSIN D

Chain D: 



#### • Molecule 3: PEPSTATIN

Chain I: 



- Molecule 3: PEPSTATIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.90Å 125.90Å 104.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, $R_{free}$	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 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: MAN, BMA, NAG, IVA, STA

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	0.85	0/771	1.47	9/1051 (0.9%)
1	C	0.87	0/771	1.56	9/1051 (0.9%)
2	B	0.77	0/1884	1.45	13/2551 (0.5%)
2	D	0.74	0/1884	1.49	17/2551 (0.7%)
3	I	0.74	0/17	1.57	0/21
3	J	0.81	0/17	2.17	1/21 (4.8%)
All	All	0.79	0/5344	1.49	49/7246 (0.7%)

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
2	D	0	1
3	I	0	2
3	J	0	2
All	All	0	6

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	C	40	TRP	CG-CD2-CE3	8.57	141.62	133.90
1	C	40	TRP	CE2-CD2-CG	-8.42	100.56	107.30
2	D	319	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	A	40	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	C	40	TRP	CB-CG-CD1	-7.80	116.86	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	319	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	54	TRP	CD1-CG-CD2	7.52	112.32	106.30
2	B	319	TRP	CE2-CD2-CG	-7.48	101.31	107.30
2	D	112	ARG	NE-CZ-NH2	-7.41	116.59	120.30
2	D	256	LEU	N-CA-C	-7.38	91.06	111.00
1	C	59	TYR	CB-CG-CD2	-7.35	116.59	121.00
1	A	40	TRP	CE2-CD2-CG	-7.28	101.47	107.30
2	D	319	TRP	CE2-CD2-CG	-7.28	101.48	107.30
2	D	112	ARG	NE-CZ-NH1	6.91	123.76	120.30
2	B	206	TRP	CD1-CG-CD2	6.80	111.74	106.30
2	D	339	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	D	206	TRP	CD1-CG-CD2	6.67	111.64	106.30
2	D	339	ARG	NE-CZ-NH2	-6.67	116.96	120.30
2	D	206	TRP	CE2-CD2-CG	-6.63	102.00	107.30
2	B	335	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	D	328	ARG	NE-CZ-NH1	6.55	123.57	120.30
2	B	206	TRP	CE2-CD2-CG	-6.20	102.34	107.30
2	B	319	TRP	CG-CD2-CE3	6.16	139.44	133.90
1	A	67	TYR	CB-CG-CD2	-6.00	117.40	121.00
2	B	182	MET	CA-CB-CG	-5.96	103.16	113.30
1	C	54	TRP	CD1-CG-CD2	5.91	111.03	106.30
2	D	192	LYS	CA-CB-CG	5.89	126.36	113.40
2	B	335	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	54	TRP	CE2-CD2-CG	-5.84	102.63	107.30
2	B	141	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	B	296	GLN	N-CA-C	-5.75	95.46	111.00
1	C	94	VAL	N-CA-C	-5.74	95.49	111.00
1	C	54	TRP	CE2-CD2-CG	-5.70	102.74	107.30
2	D	195	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	54	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	A	40	TRP	CG-CD2-CE3	5.57	138.91	133.90
2	B	340	VAL	CA-C-N	5.46	127.12	116.20
2	D	258	GLN	CA-CB-CG	5.42	125.33	113.40
2	D	319	TRP	CG-CD1-NE1	-5.38	104.72	110.10
2	D	319	TRP	CG-CD2-CE3	5.37	138.73	133.90
3	J	2	VAL	CA-CB-CG2	-5.28	102.97	110.90
1	C	80	SER	CA-C-N	5.26	126.71	116.20
2	D	208	VAL	N-CA-CB	-5.20	100.05	111.50
2	B	245	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	B	247	LEU	CB-CG-CD1	-5.15	102.24	111.00
2	D	221	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	49	LEU	CA-CB-CG	5.00	126.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	GLY	Peptide
2	D	312	PRO	Peptide
3	I	4	STA	Mainchain,Peptide
3	J	4	STA	Mainchain,Peptide

## 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	748	156	702	13	0
1	C	748	156	702	8	0
2	B	1845	389	1849	22	0
2	D	1845	389	1849	25	0
3	I	48	7	60	2	0
3	J	48	7	60	2	0
4	A	50	46	43	0	0
4	C	50	46	43	3	0
5	B	14	14	13	0	0
5	D	14	14	13	0	0
6	A	9	18	0	0	0
6	B	13	26	0	0	0
6	C	9	18	0	1	0
6	D	13	26	0	0	0
All	All	5454	1312	5334	63	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 (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:C:43:SER:HB2	2:D:117:GLU:HB3	1.58	0.84
2:D:263:ILE:HD13	2:D:271:LEU:HD21	1.78	0.64
2:B:268:VAL:HA	2:B:271:LEU:HD22	1.78	0.63
1:C:72:THR:HB	1:C:87:LEU:HD12	1.81	0.61
2:B:236:LEU:HD22	2:B:305:GLY:HA2	1.81	0.61
2:D:264:PRO:HG2	2:D:267:LYS:HG2	1.84	0.60
2:B:267:LYS:O	2:B:271:LEU:HD13	2.03	0.59
1:A:19:ILE:HG22	1:A:94:VAL:HG22	1.84	0.59
2:B:222:CYS:SG	2:B:222:CYS:O	2.61	0.58
3:J:1:IVA:O	3:J:2:VAL:HB	2.04	0.58
1:A:31:VAL:HG23	1:A:33:ASP:HB2	1.86	0.57
2:B:260:GLU:HG3	2:B:307:MET:HG3	1.88	0.56
1:A:3:ILE:HB	2:B:183:LEU:HB2	1.87	0.56
2:D:293:LYS:HE2	2:D:300:THR:HG23	1.89	0.55
2:D:221:LEU:HD11	2:D:247:LEU:HB2	1.89	0.55
2:D:281:LYS:H	2:D:281:LYS:HD2	1.72	0.54
1:A:88:SER:O	2:B:114:VAL:HA	2.08	0.53
2:B:234:THR:HG21	2:B:320:ILE:HG21	1.90	0.53
2:B:171:ARG:HD3	2:B:327:GLY:HA3	1.92	0.51
1:A:78:TYR:HE2	1:A:83:LEU:HD21	1.75	0.51
4:C:99:NAG:C3	4:C:100:BMA:O5	2.59	0.50
3:I:1:IVA:O	3:I:2:VAL:HB	2.12	0.49
2:B:151:PHE:O	2:B:155:MET:HG3	2.13	0.49
2:D:222:CYS:O	2:D:222:CYS:SG	2.71	0.48
2:B:195:LEU:HD13	2:B:343:ALA:HB2	1.95	0.48
2:B:188:SER:HA	2:B:191:TYR:CE1	2.48	0.48
2:D:237:MET:SD	2:D:325:PHE:HB2	2.55	0.47
2:B:207:GLN:HG2	2:B:229:ILE:HG22	1.97	0.47
2:D:311:ILE:HD11	2:D:320:ILE:HD11	1.97	0.47
1:A:39:LEU:HA	2:B:134:ILE:O	2.15	0.47
1:C:15:TYR:CD2	2:D:169:LEU:HD22	2.49	0.47
2:D:228:ALA:HA	2:D:319:TRP:O	2.14	0.46
1:A:89:GLN:HA	2:B:113:GLN:O	2.16	0.46
4:C:99:NAG:O7	4:C:99:NAG:C1	2.63	0.46
2:D:237:MET:HE1	2:D:276:LEU:HD21	1.98	0.45
2:D:195:LEU:HD13	2:D:343:ALA:HB2	1.99	0.45
2:B:142:ILE:HG23	2:B:204:ALA:HB1	1.99	0.45
2:D:244:VAL:O	2:D:248:GLN:HG2	2.17	0.44
2:D:236:LEU:HD11	3:J:1:IVA:HG23	1.99	0.43
1:A:80:SER:OG	3:I:2:VAL:HA	2.18	0.43
1:C:9:ASN:ND2	2:D:170:SER:O	2.52	0.43
1:C:39:LEU:HA	2:D:134:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLY:HA2	1:C:26:GLN:O	2.18	0.43
1:A:20:GLY:O	1:A:92:VAL:HA	2.18	0.43
2:B:214:GLU:HG3	2:B:275:THR:HB	2.00	0.43
2:B:207:GLN:CG	2:B:229:ILE:HG22	2.49	0.43
2:B:238:VAL:HA	2:B:307:MET:O	2.18	0.43
4:C:98:NAG:H5	4:C:99:NAG:O7	2.18	0.43
2:D:287:PRO:HA	2:D:290:TYR:CE2	2.54	0.43
2:B:316:GLY:HA2	2:B:318:LEU:HG	1.99	0.43
1:C:76:ILE:HG12	2:D:144:VAL:HG21	2.00	0.43
2:D:251:ILE:HG22	2:D:272:PRO:CG	2.49	0.42
2:D:311:ILE:O	2:D:316:GLY:HA3	2.20	0.42
2:D:144:VAL:O	2:D:147:VAL:HG23	2.18	0.42
1:A:30:VAL:HA	2:B:133:GLY:O	2.19	0.42
2:D:335:ARG:HD2	2:D:335:ARG:HA	1.84	0.41
1:A:69:LYS:HE3	1:A:69:LYS:HB2	1.84	0.41
2:D:311:ILE:HD12	2:D:318:LEU:HB2	2.02	0.41
2:B:299:LYS:O	2:B:301:LEU:N	2.54	0.41
1:A:44:ILE:HG12	1:A:59:TYR:O	2.21	0.41
1:C:89:GLN:HG2	6:C:108:HOH:O	2.21	0.40
2:D:164:ILE:HG22	2:D:334:ASP:HA	2.03	0.40
1:A:95:PRO:O	1:A:97:GLN:N	2.54	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	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
1	C	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
2	B	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	24	41
2	D	239/241 (99%)	218 (91%)	16 (7%)	5 (2%)	9	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	3/6 (50%)	2 (67%)	0	1 (33%)	0	0
3	J	3/6 (50%)	2 (67%)	0	1 (33%)	0	0
All	All	674/688 (98%)	629 (93%)	36 (5%)	9 (1%)	15	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	224	GLU
3	J	2	VAL
2	D	300	THR
2	B	258	GLN
3	I	2	VAL
2	B	300	THR
2	D	297	ALA
2	D	241	VAL
2	D	314	PRO

### 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	85/86 (99%)	80 (94%)	5 (6%)	24	44
1	C	85/86 (99%)	82 (96%)	3 (4%)	43	70
2	B	199/199 (100%)	184 (92%)	15 (8%)	17	31
2	D	199/199 (100%)	182 (92%)	17 (8%)	13	25
3	I	2/2 (100%)	0	2 (100%)	0	0
3	J	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	572/574 (100%)	529 (92%)	43 (8%)	17	31

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR

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Mol	Chain	Res	Type
1	A	73	SER
1	A	82	SER
1	A	83	LEU
1	A	93	SER
2	B	161	ASP
2	B	171	ARG
2	B	188	SER
2	B	194	SER
2	B	208	VAL
2	B	224	GLU
2	B	238	VAL
2	B	242	ASP
2	B	254	VAL
2	B	263	ILE
2	B	269	SER
2	B	277	LYS
2	B	288	GLU
2	B	295	SER
2	B	328	ARG
3	I	2	VAL
3	I	3	VAL
1	C	83	LEU
1	C	93	SER
1	C	96	CYS
2	D	108	VAL
2	D	141	ARG
2	D	166	SER
2	D	171	ARG
2	D	186	THR
2	D	208	VAL
2	D	217	SER
2	D	223	LYS
2	D	235	SER
2	D	238	VAL
2	D	277	LYS
2	D	278	LEU
2	D	281	LYS
2	D	288	GLU
2	D	299	LYS
2	D	303	LEU
2	D	328	ARG
3	J	3	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	GLN
2	D	146	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
3	STA	I	4	3	10,10,11	0.76	0	10,12,14	2.23	5 (50%)
3	STA	I	6	3	8,11,11	1.09	1 (12%)	8,14,14	2.56	4 (50%)
3	STA	J	4	3	10,10,11	0.96	0	10,12,14	2.06	5 (50%)
3	STA	J	6	3	8,11,11	1.65	2 (25%)	8,14,14	2.81	5 (62%)

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	STA	I	4	3	-	0/11/11/12	0/0/0/0
3	STA	I	6	3	-	0/10/12/12	0/0/0/0
3	STA	J	4	3	-	0/11/11/12	0/0/0/0
3	STA	J	6	3	-	0/10/12/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	6	STA	CH-CA	2.36	1.55	1.53
3	I	6	STA	CH-CA	2.38	1.55	1.53
3	J	6	STA	CM-CH	3.91	1.57	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	6	STA	OH-CH-CM	-4.12	102.56	109.73
3	J	4	STA	OH-CH-CM	-3.37	101.52	109.34
3	I	6	STA	OH-CH-CA	-3.33	104.56	109.49
3	J	6	STA	CB-CA-N	-3.08	100.29	109.13
3	I	6	STA	OH-CH-CM	-3.06	104.42	109.73
3	J	6	STA	OH-CH-CA	-2.89	105.21	109.49
3	I	4	STA	OH-CH-CM	-2.85	102.72	109.34
3	J	4	STA	CH-CM-C	-2.53	109.45	113.27
3	I	4	STA	OH-CH-CA	-2.41	105.92	109.49
3	J	4	STA	OH-CH-CA	-2.36	106.00	109.49
3	I	4	STA	CH-CM-C	-2.23	109.90	113.27
3	J	4	STA	O-C-CM	-2.15	117.41	125.24
3	J	6	STA	CG-CB-CA	2.61	121.53	115.77
3	I	6	STA	CM-CH-CA	2.85	117.02	112.68
3	J	4	STA	CM-CH-CA	3.05	117.33	112.68
3	I	4	STA	CM-CH-CA	3.27	117.66	112.68
3	I	4	STA	CG-CB-CA	4.00	124.60	115.77
3	J	6	STA	CM-CH-CA	4.49	119.52	112.68
3	I	6	STA	CG-CB-CA	4.56	125.84	115.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected



value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	BMA	A	100	4	11,11,12	1.85	3 (27%)	14,15,17	1.95	5 (35%)
4	MAN	A	101	4	11,11,12	1.16	2 (18%)	14,15,17	1.13	1 (7%)
4	NAG	A	98	1,4	14,14,15	0.65	0	15,19,21	1.40	2 (13%)
4	NAG	A	99	4	14,14,15	0.52	0	15,19,21	1.38	2 (13%)
4	BMA	C	100	4	11,11,12	0.79	0	14,15,17	1.82	5 (35%)
4	MAN	C	101	4	11,11,12	0.82	0	14,15,17	1.72	3 (21%)
4	NAG	C	98	1,4	14,14,15	0.74	0	15,19,21	1.68	3 (20%)
4	NAG	C	99	4	14,14,15	0.76	0	15,19,21	2.19	8 (53%)

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	BMA	A	100	4	-	0/2/19/22	1/1/1/1
4	MAN	A	101	4	-	0/2/19/22	1/1/1/1
4	NAG	A	98	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	99	4	-	0/6/23/26	0/1/1/1
4	BMA	C	100	4	-	0/2/19/22	0/1/1/1
4	MAN	C	101	4	-	0/2/19/22	0/1/1/1
4	NAG	C	98	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	99	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	101	MAN	O5-C1	2.22	1.47	1.43
4	A	101	MAN	C2-C3	2.23	1.55	1.52
4	A	100	BMA	O3-C3	2.80	1.49	1.43
4	A	100	BMA	C4-C3	2.90	1.60	1.52
4	A	100	BMA	C4-C5	3.49	1.60	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	100	BMA	C2-C3-C4	-4.00	104.25	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	98	NAG	C2-N2-C7	-3.95	117.96	123.04
4	A	100	BMA	C1-C2-C3	-3.04	105.95	109.54
4	C	99	NAG	O3-C3-C2	-2.91	103.35	109.11
4	C	101	MAN	C3-C4-C5	-2.77	105.36	110.20
4	A	99	NAG	O4-C4-C3	-2.72	104.22	110.34
4	C	100	BMA	O3-C3-C4	-2.70	104.25	110.34
4	C	98	NAG	C3-C4-C5	-2.65	105.58	110.20
4	C	100	BMA	C1-C2-C3	-2.56	106.51	109.54
4	C	99	NAG	C4-C3-C2	-2.53	107.29	111.23
4	C	99	NAG	C3-C4-C5	-2.49	105.86	110.20
4	C	99	NAG	C3-C2-N2	-2.34	104.96	110.56
4	A	98	NAG	C4-C3-C2	-2.02	108.09	111.23
4	A	100	BMA	O3-C3-C4	2.11	115.10	110.34
4	C	100	BMA	C2-C3-C4	2.15	114.69	111.04
4	C	99	NAG	C6-C5-C4	2.16	118.35	113.02
4	C	99	NAG	O7-C7-N2	2.24	126.44	121.86
4	A	100	BMA	O5-C1-C2	2.38	114.72	110.86
4	A	101	MAN	C1-O5-C5	2.41	115.30	112.25
4	C	98	NAG	O4-C4-C5	2.52	115.93	109.24
4	A	99	NAG	C3-C4-C5	2.54	114.62	110.20
4	C	99	NAG	C2-N2-C7	2.65	126.45	123.04
4	C	101	MAN	C1-C2-C3	2.76	112.81	109.54
4	C	100	BMA	C1-O5-C5	2.92	115.95	112.25
4	A	100	BMA	O2-C2-C1	3.02	115.26	109.21
4	C	101	MAN	C6-C5-C4	3.40	121.39	113.02
4	C	100	BMA	O2-C2-C1	3.53	116.28	109.21
4	C	99	NAG	O4-C4-C3	4.50	120.46	110.34
4	C	98	NAG	C1-O5-C5	4.73	118.25	112.25

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	MAN	C1-C2-C3-C4-C5-O5
4	A	100	BMA	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	100	BMA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	98	NAG	1	0
4	C	99	NAG	3	0

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	1	2	14,14,15	1.43	2 (14%)	15,19,21	1.46	4 (26%)
5	NAG	D	1	2	14,14,15	1.56	2 (14%)	15,19,21	2.08	4 (26%)

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
5	NAG	B	1	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	NAG	C3-C2	2.42	1.58	1.52
5	D	1	NAG	O5-C1	2.49	1.47	1.43
5	B	1	NAG	C1-C2	3.66	1.57	1.52
5	D	1	NAG	C1-C2	4.43	1.58	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1	NAG	C4-C3-C2	-2.87	106.76	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	C4-C3-C2	-2.69	107.04	111.23
5	D	1	NAG	C3-C4-C5	-2.34	106.11	110.20
5	B	1	NAG	C3-C4-C5	-2.03	106.66	110.20
5	D	1	NAG	O4-C4-C5	2.01	114.56	109.24
5	B	1	NAG	O3-C3-C2	2.29	113.65	109.11
5	B	1	NAG	C1-O5-C5	2.75	115.73	112.25
5	D	1	NAG	C1-O5-C5	6.20	120.11	112.25

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.