



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:18 AM UTC

PDB ID : 1LYW / pdb_00001lyw
Title : CATHEPSIN D AT PH 7.5
Authors : Lee, A.Y.; Gulnik, S.V.; Erickson, J.W.
Deposited on : 1998-06-30
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

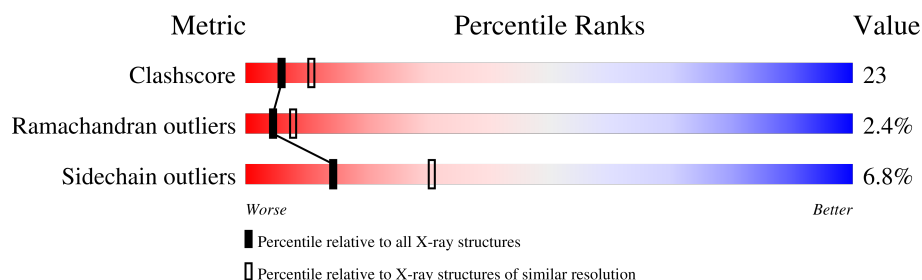
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	97	57% 34% 7% .
1	C	97	42% 54% . .
1	E	97	56% 37% 5% .
1	G	97	42% 47% 7% . .
2	B	241	54% 42% .
2	D	241	52% 41% 6%
2	F	241	45% 51% . .
2	H	241	50% 47% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EPE	C	98	-	-	X	-
3	EPE	G	98	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14242 atoms, of which 3296 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.

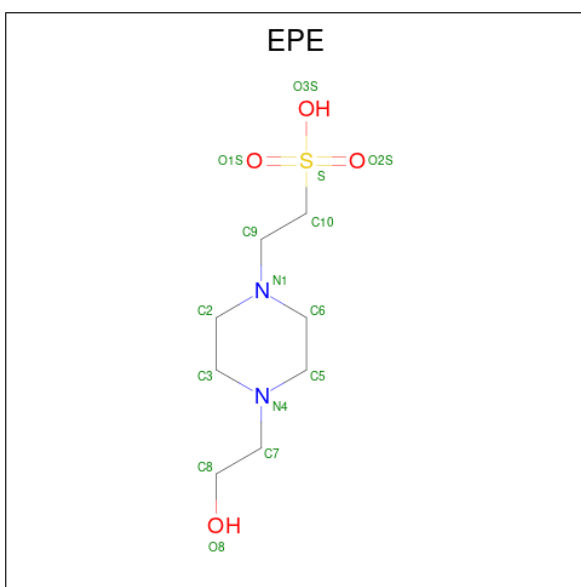
- Molecule 1 is a protein called CATHEPSIN D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	95	Total	C	H	N	O	S	0	0	0
			890	471	153	117	144	5			
1	C	95	Total	C	H	N	O	S	0	0	0
			890	471	153	117	144	5			
1	E	95	Total	C	H	N	O	S	0	0	0
			890	471	153	117	144	5			
1	G	95	Total	C	H	N	O	S	0	0	0
			890	471	153	117	144	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
			2235	1184	390	302	348	11			
2	D	241	Total	C	H	N	O	S	0	0	0
			2235	1184	390	302	348	11			
2	F	241	Total	C	H	N	O	S	0	0	0
			2235	1184	390	302	348	11			
2	H	241	Total	C	H	N	O	S	0	0	0
			2235	1184	390	302	348	11			

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			17	8	2	2	4	1		
3	C	1	Total	C	H	N	O	S	0	0
			17	8	2	2	4	1		
3	E	1	Total	C	H	N	O	S	0	0
			17	8	2	2	4	1		
3	G	1	Total	C	H	N	O	S	0	0
			17	8	2	2	4	1		

- Molecule 4 is water.

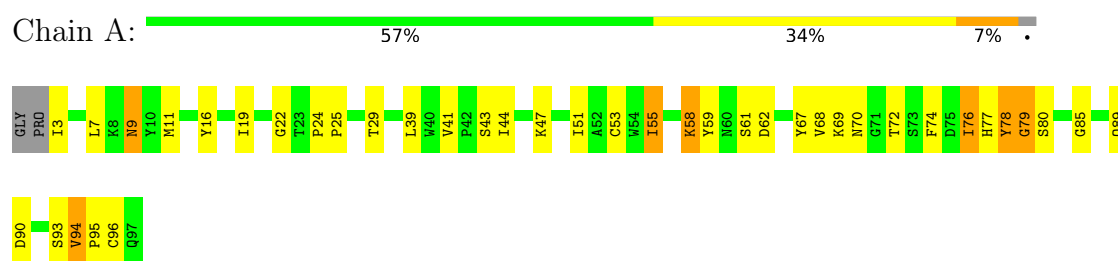
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	55	Total	H	O	0	0
			165	110	55		
4	B	110	Total	H	O	0	0
			330	220	110		
4	C	55	Total	H	O	0	0
			165	110	55		
4	D	78	Total	H	O	0	0
			234	156	78		
4	E	46	Total	H	O	0	0
			138	92	46		
4	F	90	Total	H	O	0	0
			270	180	90		
4	G	39	Total	H	O	0	0
			117	78	39		
4	H	85	Total	H	O	0	0
			255	170	85		

3 Residue-property plots

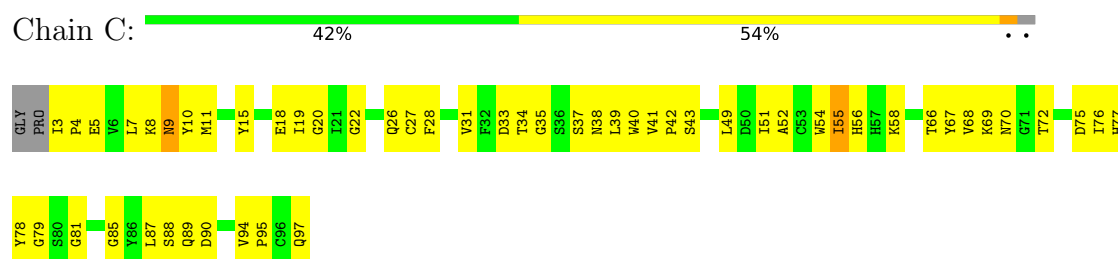
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

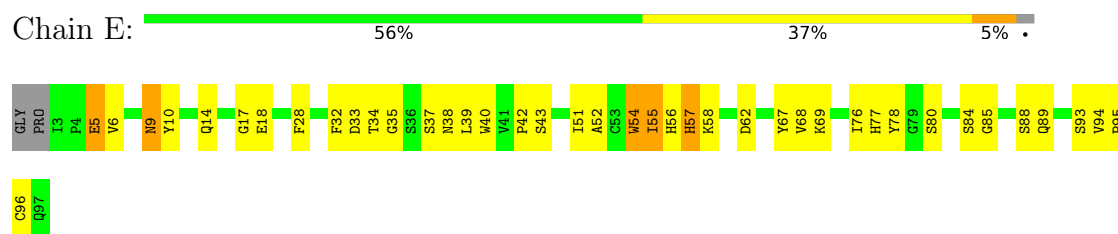
• Molecule 1: CATHEPSIN D



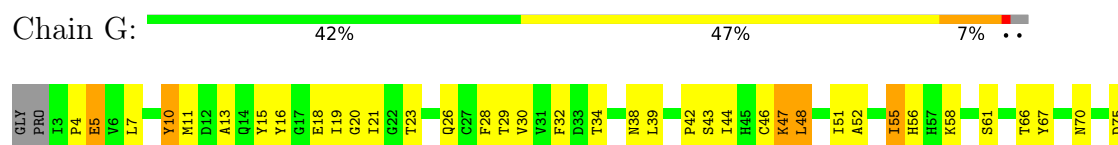
• Molecule 1: CATHEPSIN D



• Molecule 1: CATHEPSIN D



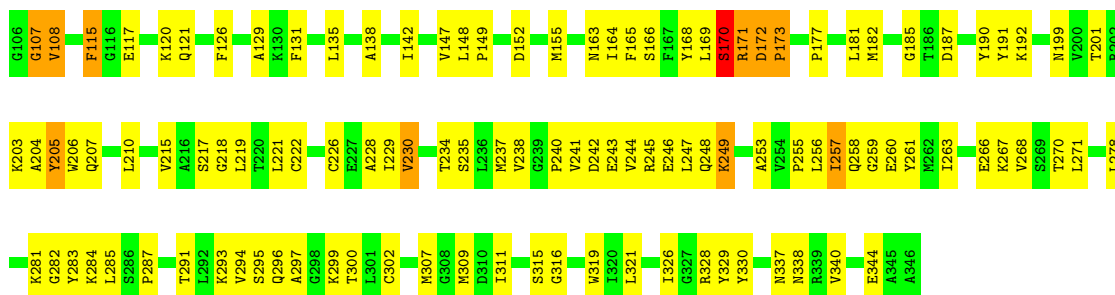
• Molecule 1: CATHEPSIN D





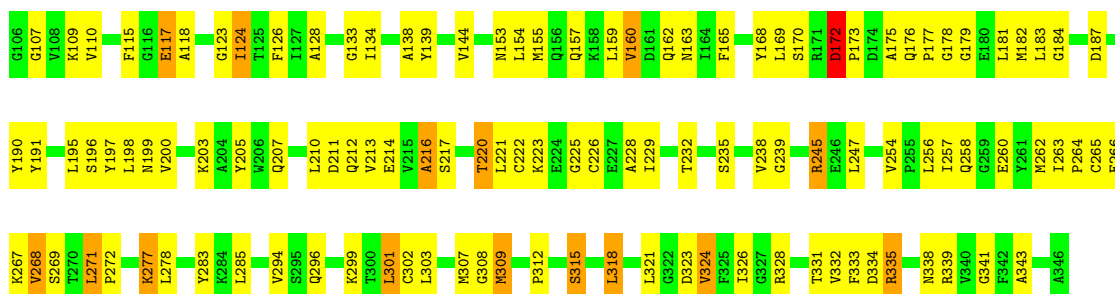
• Molecule 2: CATHEPSIN D

Chain B: 54% 42%



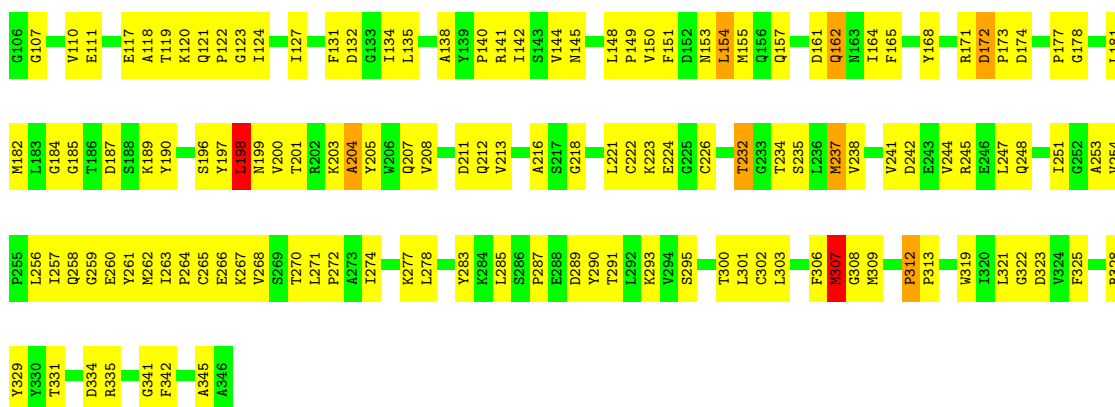
• Molecule 2: CATHEPSIN D

Chain D: 52% 41% 6%



• Molecule 2: CATHEPSIN D

Chain F: 45% 51%



• Molecule 2: CATHEPSIN D

Chain H: 50% 47%

A345	E260	L181	G106
A346	M261	M182	G107
	G262	L183	V108
	P264	G184	K109
	C265	S188	V110
	E266	Y191	E111
	K267		R112
	V268		F115
		S196	G116
	L271	Y197	E117
	P272	L198	A118
	K277	R202	T119
	L278		K120
	G279	Y205	Q121
	G280	W206	P122
		Q207	G123
			T124
	Y283		T125
	K284	L210	F126
	L285	D111	T127
		Q212	A128
	Y290		A129
		V215	
	L301	A216	D132
	C302		G133
	L303	L219	I134
		T220	
	M307	L221	S143
	G308	C222	V144
	M309	K223	M145
	D310		N146
	L311	C226	V147
	P312	E227	
	P313	A228	F151
	F314	I229	D152
	S315	V230	M153
		D231	L154
	L318	T232	M155
	M319	G233	Q156
	I320	T234	Q157
	L321		K158
	G322	M237	L159
	D323	V238	V160
	P324		D161
	F325	V241	Q162
	I326	D242	N163
		E243	T164
	Y330	V244	F165
		R245	S166
	R335	E246	F167
	D336	L247	Y168
	N337	Q248	L169
	M338	K249	
	R339		A175
	V340	A253	Q176
	G341	V254	P177
	F342	P255	G178
	A343	L256	V179
	F344		S180

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.26 Å 136.80 Å 140.42 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	73.0 (8.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.195 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14242	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: EPE

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	0.58	0/759	1.03	0/1034
1	C	0.57	0/759	1.03	2/1034 (0.2%)
1	E	0.62	0/759	1.03	2/1034 (0.2%)
1	G	0.64	0/759	1.08	5/1034 (0.5%)
2	B	0.66	0/1884	1.12	16/2551 (0.6%)
2	D	0.66	1/1884 (0.1%)	1.18	10/2551 (0.4%)
2	F	0.66	1/1884 (0.1%)	1.09	12/2551 (0.5%)
2	H	0.63	0/1884	1.07	8/2551 (0.3%)
All	All	0.64	2/10572 (0.0%)	1.10	55/14340 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	335	ARG	CZ-NH1	6.44	1.41	1.32
2	F	335	ARG	CZ-NH1	5.53	1.40	1.32

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	257	ILE	N-CA-C	-8.27	100.87	110.21
1	E	57	HIS	N-CA-C	-7.56	100.77	110.53
2	D	123	GLY	N-CA-C	7.45	124.73	112.66
2	D	324	VAL	N-CA-C	-7.43	103.28	110.42
2	D	257	ILE	N-CA-C	7.40	118.13	110.36

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	737	153	690	40	0
1	C	737	153	690	59	0
1	E	737	153	690	43	0
1	G	737	153	690	51	0
2	B	1845	390	1850	92	0
2	D	1845	390	1850	88	0
2	F	1845	390	1850	92	0
2	H	1845	390	1850	94	0
3	A	15	2	18	4	0
3	C	15	2	18	8	0
3	E	15	2	18	2	0
3	G	15	2	18	11	0
4	A	55	110	0	0	0
4	B	110	220	0	0	0
4	C	55	110	0	2	0
4	D	78	156	0	0	0
4	E	46	92	0	0	0
4	F	90	180	0	2	0
4	G	39	78	0	0	0
4	H	85	170	0	2	0
All	All	10946	3296	10232	473	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 23.

The worst 5 of 473 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:G:7:LEU:HD11	2:H:309:MET:HG2	1.29	1.05
2:H:253:ALA:HB1	2:H:261:TYR:HB3	1.39	1.04
1:E:43:SER:HB2	2:F:117:GLU:HG2	1.39	1.03
1:G:83:LEU:HD23	3:G:98:EPE:H92	1.42	1.02
2:B:172:ASP:HB2	2:B:173:PRO:HD3	1.44	1.00

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	93/97 (96%)	80 (86%)	10 (11%)	3 (3%)	3	4
1	C	93/97 (96%)	83 (89%)	9 (10%)	1 (1%)	11	22
1	E	93/97 (96%)	83 (89%)	9 (10%)	1 (1%)	11	22
1	G	93/97 (96%)	79 (85%)	12 (13%)	2 (2%)	5	9
2	B	239/241 (99%)	209 (87%)	23 (10%)	7 (3%)	3	5
2	D	239/241 (99%)	215 (90%)	18 (8%)	6 (2%)	4	7
2	F	239/241 (99%)	218 (91%)	13 (5%)	8 (3%)	3	4
2	H	239/241 (99%)	211 (88%)	24 (10%)	4 (2%)	7	13
All	All	1328/1352 (98%)	1178 (89%)	118 (9%)	32 (2%)	4	8

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
2	B	171	ARG
2	B	173	PRO
1	C	9	ASN
2	D	216	ALA

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	84/86 (98%)	75 (89%)	9 (11%)	6	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	84/86 (98%)	82 (98%)	2 (2%)	43	70
1	E	84/86 (98%)	79 (94%)	5 (6%)	17	36
1	G	84/86 (98%)	71 (84%)	13 (16%)	2	5
2	B	199/199 (100%)	188 (94%)	11 (6%)	19	40
2	D	199/199 (100%)	184 (92%)	15 (8%)	12	26
2	F	199/199 (100%)	186 (94%)	13 (6%)	15	32
2	H	199/199 (100%)	190 (96%)	9 (4%)	24	49
All	All	1132/1140 (99%)	1055 (93%)	77 (7%)	14	31

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	29	THR
2	H	162	GLN
1	G	47	LYS
1	G	93	SER
2	H	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	56	HIS
2	H	199	ASN
2	H	338	ASN
2	H	337	ASN
2	D	153	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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$
3	EPE	A	98	-	15,15,15	1.18	2 (13%)	19,20,20	2.29	8 (42%)
3	EPE	G	98	-	15,15,15	0.86	1 (6%)	19,20,20	1.93	5 (26%)
3	EPE	E	98	-	15,15,15	1.23	2 (13%)	19,20,20	2.22	7 (36%)
3	EPE	C	98	-	15,15,15	1.34	2 (13%)	19,20,20	2.33	6 (31%)

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	EPE	A	98	-	-	1/9/19/19	0/1/1/1
3	EPE	G	98	-	-	1/9/19/19	0/1/1/1
3	EPE	E	98	-	-	4/9/19/19	0/1/1/1
3	EPE	C	98	-	-	6/9/19/19	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	98	EPE	O3S-S	3.59	1.60	1.47
3	C	98	EPE	C10-S	3.44	1.82	1.77
3	E	98	EPE	O3S-S	3.38	1.59	1.47
3	E	98	EPE	C10-S	2.91	1.81	1.77
3	A	98	EPE	O3S-S	2.69	1.57	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	98	EPE	C5-N4-C3	-5.50	96.99	108.84
3	C	98	EPE	C5-N4-C3	-5.10	97.84	108.84
3	C	98	EPE	O3S-S-O2S	-4.51	100.11	111.40
3	C	98	EPE	C3-C2-N1	4.51	119.74	110.65
3	A	98	EPE	O3S-S-C10	3.98	113.80	106.00

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	98	EPE	C10-C9-N1-C6
3	C	98	EPE	C9-C10-S-O2S
3	C	98	EPE	C9-C10-S-O3S
3	C	98	EPE	C8-C7-N4-C3
3	E	98	EPE	C9-C10-S-O3S

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	98	EPE	4	0
3	G	98	EPE	11	0
3	E	98	EPE	2	0
3	C	98	EPE	8	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

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.