



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:55 PM UTC

PDB ID : 1X8K / pdb_00001x8k
Title : Crystal structure of retinol dehydratase in complex with anhydroretinol and inactive cofactor PAP
Authors : Pakhomova, S.; Buck, J.; Newcomer, M.E.
Deposited on : 2004-08-18
Resolution : 2.75 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

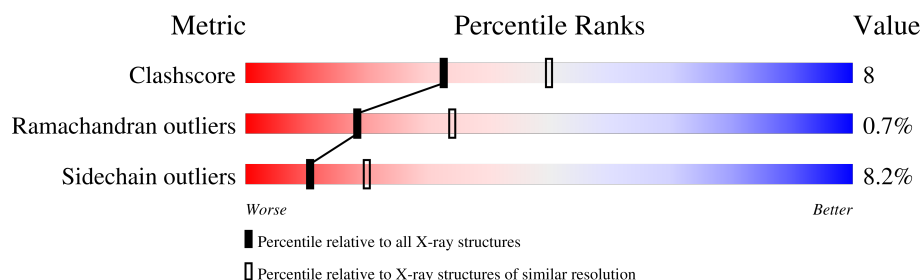
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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	351	 76% 20% . .
1	B	351	 69% 26% . .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5872 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.

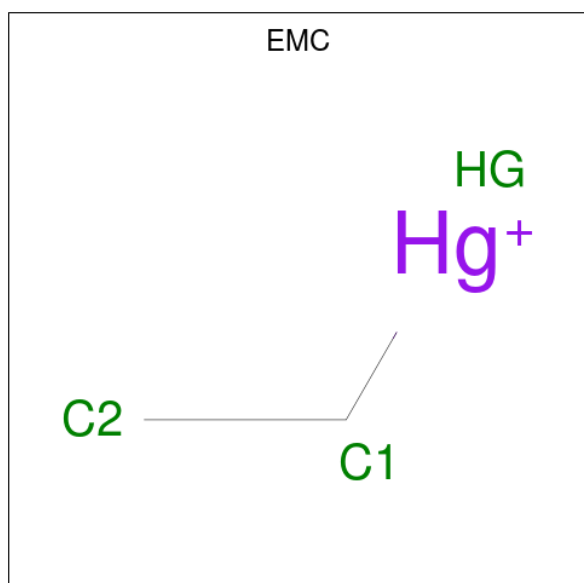
- Molecule 1 is a protein called retinol dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2850	1844	471	520	15			
1	B	344	Total	C	N	O	S	0	0	0
			2846	1842	471	518	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	PHE	SEE REMARK 999	UNP Q26490
A	258	SER	CYS	engineered mutation	UNP Q26490
A	279	SER	CYS	engineered mutation	UNP Q26490
B	142	SER	PHE	SEE REMARK 999	UNP Q26490
B	258	SER	CYS	engineered mutation	UNP Q26490
B	279	SER	CYS	engineered mutation	UNP Q26490

- Molecule 2 is ETHYL MERCURY ION (CCD ID: EMC) (formula: $\text{C}_2\text{H}_5\text{Hg}$).

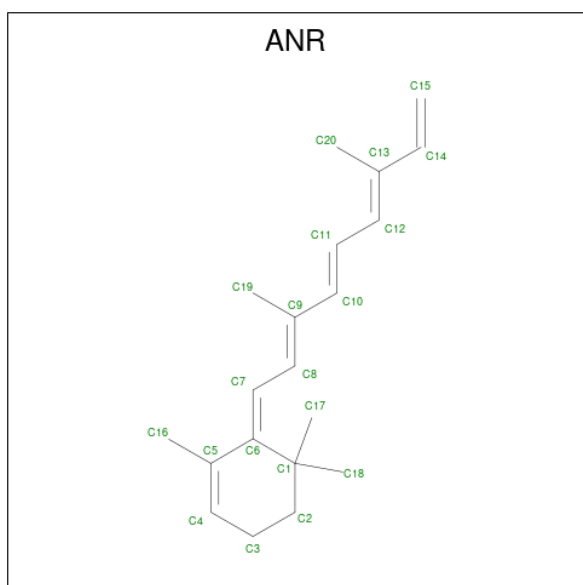


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	B	1	Total	C	Hg	0	0
			3	2	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

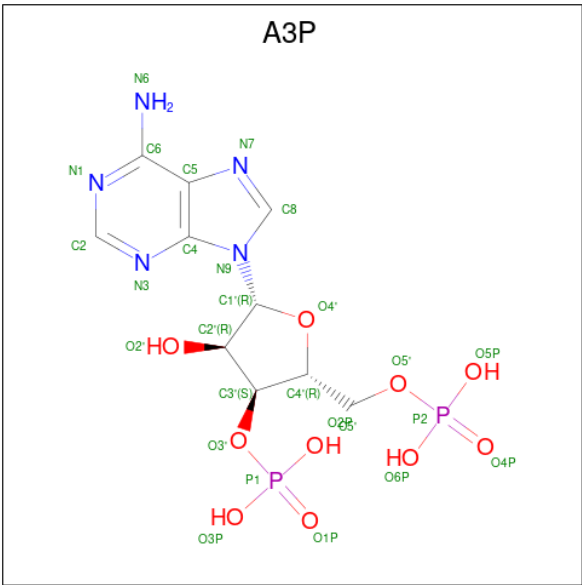
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ANHYDRORETINOL (CCD ID: ANR) (formula: C₂₀H₂₈).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			20	20		
4	B	1	Total	C	0	0
			20	20		

- Molecule 5 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		
6	B	33	Total	O	0	0
			33	33		

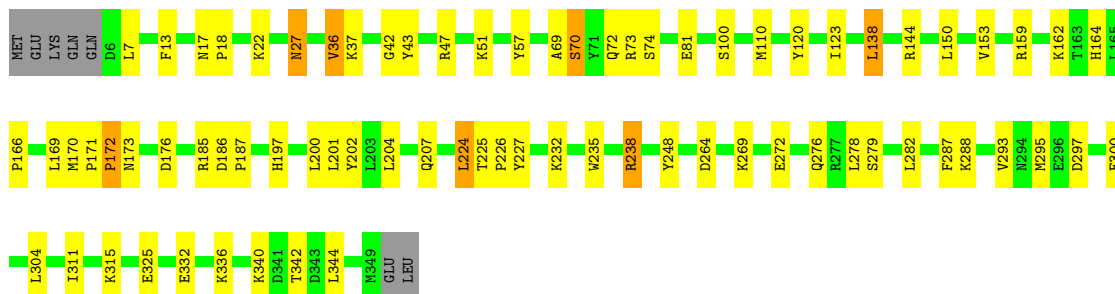
3 Residue-property plots [i](#)

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. 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.

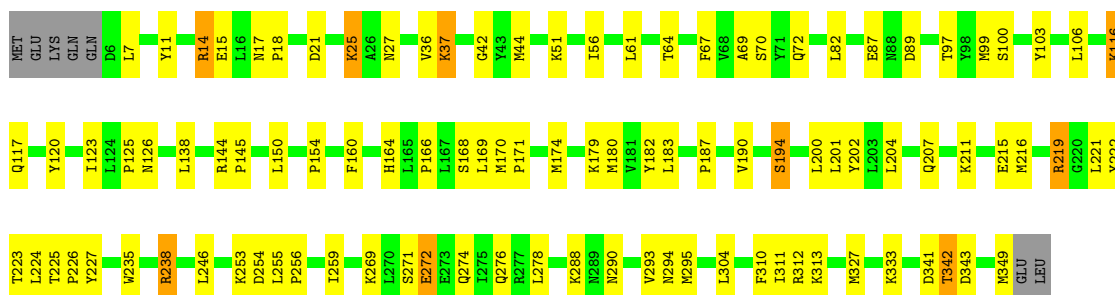
- Molecule 1: retinol dehydratase

Chain A: 



- Molecule 1: retinol dehydratase

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.29Å 66.66Å 84.46Å 90.00° 110.66° 90.00°	Depositor
Resolution (Å)	15.00 – 2.75	Depositor
% Data completeness (in resolution range)	95.5 (15.00-2.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5872	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: A3P, CA, ANR, EMC

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	0.67	0/2931	0.99	1/3969 (0.0%)
1	B	0.68	0/2927	1.00	1/3964 (0.0%)
All	All	0.68	0/5858	1.00	2/7933 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	PRO	O-C-N	5.24	123.72	121.31
1	A	172	PRO	N-CA-C	-5.02	103.30	111.68

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	2850	0	2774	36	0
1	B	2846	0	2770	53	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	20	0	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	28	1	0
5	B	54	0	22	1	0
6	A	41	0	0	1	0
6	B	33	0	0	3	0
All	All	5872	0	5622	90	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 8.

All (90) 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:120:TYR:O	1:A:123:ILE:HG12	1.85	0.75
1:B:215:GLU:O	1:B:219:ARG:HB2	1.92	0.70
1:B:225:THR:HB	1:B:226:PRO:HA	1.75	0.69
1:A:27:ASN:O	1:A:204:LEU:HD12	1.94	0.68
1:B:37:LYS:HD3	1:B:44:MET:SD	2.36	0.66
1:B:125:PRO:C	1:B:126:ASN:HD22	2.04	0.66
1:A:225:THR:HB	1:A:226:PRO:HA	1.78	0.65
1:B:294:ASN:HA	1:B:311:ILE:HD12	1.79	0.64
1:B:21:ASP:O	1:B:25:LYS:HB2	1.98	0.62
1:B:27:ASN:O	1:B:204:LEU:HD12	2.01	0.60
1:B:187:PRO:HG3	1:B:227:TYR:CE2	2.37	0.60
1:B:235:TRP:O	1:B:238:ARG:HB3	2.02	0.60
1:B:310:PHE:CE1	4:B:2202:ANR:H203	2.37	0.60
1:A:153:VAL:HG11	1:A:159:ARG:HG2	1.86	0.58
1:B:290:ASN:HB3	1:B:293:VAL:HG22	1.85	0.58
1:B:190:VAL:O	1:B:194:SER:HB2	2.04	0.57
1:B:14:ARG:HH11	1:B:14:ARG:HG3	1.70	0.56
1:A:288:LYS:HG3	1:A:311:ILE:HG22	1.87	0.56
1:B:238:ARG:NH2	1:B:343:ASP:OD2	2.37	0.56
1:A:73:ARG:HD2	5:B:1101:A3P:O4P	2.05	0.56
1:B:87:GLU:HA	1:B:87:GLU:OE2	2.06	0.56
1:A:187:PRO:HG3	1:A:227:TYR:CE2	2.41	0.55
1:A:235:TRP:O	1:A:238:ARG:HB3	2.07	0.55
1:B:200:LEU:HD11	1:B:304:LEU:HD22	1.90	0.54
1:B:255:LEU:HB3	1:B:256:PRO:HD3	1.90	0.54
1:B:37:LYS:HD2	1:B:42:GLY:O	2.07	0.53
1:B:17:ASN:HB2	1:B:18:PRO:HD2	1.91	0.52
1:A:17:ASN:HB2	1:A:18:PRO:HD2	1.92	0.52
1:A:72:GLN:HA	1:A:164:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TYR:HA	1:A:225:THR:O	2.10	0.51
1:A:173:ASN:O	1:A:176:ASP:HB2	2.10	0.51
1:A:69:ALA:O	1:A:70:SER:HB3	2.09	0.51
1:B:120:TYR:O	1:B:123:ILE:HG12	2.11	0.50
1:B:61:LEU:CD1	1:B:174:MET:HB2	2.41	0.50
1:B:14:ARG:NH1	1:B:15:GLU:O	2.46	0.49
1:A:201:LEU:O	1:A:202:TYR:HB2	2.13	0.49
1:A:332:GLU:O	1:A:336:LYS:HB2	2.13	0.48
1:B:201:LEU:O	1:B:202:TYR:HB2	2.14	0.48
1:A:81:GLU:HG2	1:A:287:PHE:HE1	1.80	0.47
1:B:341:ASP:O	1:B:342:THR:HB	2.13	0.47
1:B:14:ARG:HG3	1:B:14:ARG:NH1	2.28	0.47
1:A:166:PRO:HD2	1:A:169:LEU:HD12	1.96	0.47
1:B:17:ASN:HB2	1:B:18:PRO:CD	2.46	0.46
1:B:56:ILE:HG12	1:B:106:LEU:HD11	1.98	0.46
1:B:103:TYR:CE2	1:B:160:PHE:HB3	2.50	0.46
1:A:197:HIS:O	1:A:200:LEU:HB3	2.17	0.45
4:A:1102:ANR:H161	4:A:1102:ANR:H7	1.79	0.45
1:B:69:ALA:O	1:B:182:TYR:HA	2.16	0.45
1:A:325:GLU:H	1:A:325:GLU:CD	2.24	0.45
1:B:225:THR:HA	1:B:226:PRO:C	2.43	0.44
1:B:67:PHE:O	1:B:180:MET:HA	2.18	0.44
1:B:72:GLN:HA	1:B:164:HIS:CE1	2.53	0.44
1:B:288:LYS:HG3	1:B:311:ILE:HG22	1.99	0.44
1:A:200:LEU:HD11	1:A:304:LEU:HD13	1.99	0.44
1:A:225:THR:HB	1:A:226:PRO:CA	2.44	0.44
1:B:37:LYS:HE3	1:B:221:LEU:HD23	2.00	0.44
1:B:97:THR:HA	6:B:2210:HOH:O	2.18	0.44
1:A:170:MET:HB3	1:A:171:PRO:CD	2.48	0.43
1:A:171:PRO:HA	1:A:172:PRO:HD3	1.95	0.43
1:B:166:PRO:HD2	1:B:169:LEU:HD12	2.00	0.43
1:B:222:TYR:CG	1:B:223:THR:N	2.87	0.43
1:B:11:TYR:HE1	1:B:168:SER:O	2.02	0.42
1:B:225:THR:HB	1:B:226:PRO:CA	2.45	0.42
1:A:185:ARG:O	1:A:186:ASP:C	2.62	0.42
1:B:15:GLU:HA	6:B:2208:HOH:O	2.18	0.42
1:A:238:ARG:NH1	6:A:1106:HOH:O	2.52	0.42
1:A:74:SER:O	1:A:248:TYR:HB2	2.19	0.42
1:A:13:PHE:HB2	1:A:36:VAL:CG1	2.50	0.42
1:B:82:LEU:HD22	1:B:259:ILE:HG12	2.02	0.42
1:A:57:TYR:O	1:A:171:PRO:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:TYR:CD2	1:B:160:PHE:HB3	2.55	0.42
1:A:342:THR:HG23	1:A:344:LEU:H	1.85	0.41
1:B:70:SER:O	1:B:164:HIS:HA	2.19	0.41
1:B:170:MET:O	1:B:171:PRO:C	2.63	0.41
1:A:278:LEU:HA	1:A:278:LEU:HD23	1.86	0.41
1:B:27:ASN:HB2	1:B:216:MET:HE1	2.03	0.41
1:A:138:LEU:HD13	1:A:138:LEU:HA	1.89	0.41
1:B:99:MET:HE2	1:B:293:VAL:HG12	2.03	0.41
1:A:37:LYS:HD3	1:A:42:GLY:O	2.20	0.41
1:B:183:LEU:HD13	1:B:246:LEU:O	2.20	0.41
1:A:110:MET:HE1	1:A:224:LEU:CD2	2.51	0.41
1:B:144:ARG:HA	1:B:145:PRO:HD2	1.94	0.41
1:B:254:ASP:OD2	6:B:2219:HOH:O	2.22	0.41
1:A:162:LYS:NZ	4:A:1102:ANR:H202	2.36	0.40
1:B:271:SER:OG	1:B:274:GLN:HG3	2.22	0.40
1:B:116:LYS:O	1:B:117:GLN:C	2.65	0.40
1:B:278:LEU:HD23	1:B:278:LEU:HA	1.77	0.40
1:A:225:THR:HA	1:A:226:PRO:C	2.47	0.40
1:A:287:PHE:CZ	1:A:293:VAL:HG21	2.56	0.40
1:B:211:LYS:HG3	1:B:327:MET:SD	2.61	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	342/351 (97%)	324 (95%)	16 (5%)	2 (1%)	21	38
1	B	342/351 (97%)	325 (95%)	14 (4%)	3 (1%)	14	28
All	All	684/702 (97%)	649 (95%)	30 (4%)	5 (1%)	18	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	LEU
1	A	70	SER
1	A	7	LEU
1	B	272	GLU
1	B	342	THR

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	305/316 (96%)	281 (92%)	24 (8%)	11	21
1	B	304/316 (96%)	278 (91%)	26 (9%)	10	18
All	All	609/632 (96%)	559 (92%)	50 (8%)	10	20

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	27	ASN
1	A	36	VAL
1	A	47	ARG
1	A	51	LYS
1	A	100	SER
1	A	138	LEU
1	A	144	ARG
1	A	150	LEU
1	A	207	GLN
1	A	224	LEU
1	A	232	LYS
1	A	238	ARG
1	A	264	ASP
1	A	269	LYS
1	A	272	GLU
1	A	276	GLN
1	A	279	SER
1	A	282	LEU

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Mol	Chain	Res	Type
1	A	295	MET
1	A	297	ASP
1	A	300	GLU
1	A	315	LYS
1	A	340	LYS
1	B	14	ARG
1	B	25	LYS
1	B	36	VAL
1	B	37	LYS
1	B	51	LYS
1	B	64	THR
1	B	89	ASP
1	B	100	SER
1	B	116	LYS
1	B	138	LEU
1	B	150	LEU
1	B	179	LYS
1	B	194	SER
1	B	207	GLN
1	B	219	ARG
1	B	224	LEU
1	B	238	ARG
1	B	253	LYS
1	B	269	LYS
1	B	272	GLU
1	B	276	GLN
1	B	295	MET
1	B	312	ARG
1	B	313	LYS
1	B	333	LYS
1	B	349	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	72	GLN
1	A	80	GLN
1	B	27	ASN
1	B	80	GLN
1	B	126	ASN
1	B	129	ASN

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Mol	Chain	Res	Type
1	B	164	HIS
1	B	173	ASN
1	B	207	GLN
1	B	283	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are 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	ANR	B	2202	-	19,20,20	3.70	8 (42%)	20,27,27	3.52	12 (60%)
5	A3P	B	2201	-	29,29,29	1.39	3 (10%)	44,45,45	2.17	14 (31%)
2	EMC	B	2203	1	1,2,2	0.55	0	-		
4	ANR	A	1102	-	19,20,20	3.58	8 (42%)	20,27,27	3.38	13 (65%)
5	A3P	B	1101	-	29,29,29	1.49	3 (10%)	44,45,45	2.04	15 (34%)
2	EMC	A	1103	1	1,2,2	0.50	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
5	A3P	B	1101	-	-	3/15/31/31	0/3/3/3
5	A3P	B	2201	-	-	2/15/31/31	0/3/3/3
4	ANR	A	1102	-	-	3/13/30/30	0/1/1/1
4	ANR	B	2202	-	-	4/13/30/30	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2202	ANR	C5-C6	-10.16	1.38	1.47
4	B	2202	ANR	C1-C6	9.80	1.66	1.53
4	A	1102	ANR	C1-C6	9.56	1.66	1.53
4	A	1102	ANR	C5-C6	-9.31	1.39	1.47
5	B	1101	A3P	C4-N3	5.44	1.44	1.34
5	B	2201	A3P	C4-N3	4.85	1.43	1.34
4	B	2202	ANR	C10-C9	-3.70	1.38	1.46
4	A	1102	ANR	C10-C9	-3.57	1.38	1.46
5	B	1101	A3P	C4-N9	-2.90	1.31	1.37
4	A	1102	ANR	C7-C6	2.85	1.41	1.36
4	B	2202	ANR	C7-C6	2.85	1.41	1.36
5	B	2201	A3P	C8-N7	2.82	1.37	1.31
5	B	2201	A3P	C4-N9	-2.82	1.31	1.37
4	A	1102	ANR	C19-C9	2.79	1.56	1.50
4	A	1102	ANR	C20-C13	2.79	1.56	1.50
4	B	2202	ANR	C20-C13	2.66	1.56	1.50
5	B	1101	A3P	C8-N7	2.62	1.36	1.31
4	B	2202	ANR	C19-C9	2.55	1.56	1.50
4	A	1102	ANR	C16-C5	2.39	1.56	1.50
4	A	1102	ANR	C4-C5	2.30	1.36	1.33
4	B	2202	ANR	C4-C5	2.23	1.36	1.33
4	B	2202	ANR	C16-C5	2.16	1.55	1.50

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2202	ANR	C16-C5-C4	-6.96	110.96	123.17
4	A	1102	ANR	C16-C5-C4	-6.95	110.98	123.17
4	A	1102	ANR	C2-C1-C6	6.16	119.38	110.44
4	B	2202	ANR	C2-C1-C6	6.10	119.31	110.44
4	A	1102	ANR	C16-C5-C6	5.57	127.66	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2201	A3P	C5-C4-N9	5.43	111.73	105.81
4	B	2202	ANR	C16-C5-C6	5.36	127.34	119.19
5	B	2201	A3P	O4'-C1'-N9	5.03	117.74	108.09
5	B	1101	A3P	C5-C4-N9	4.61	110.84	105.81
5	B	2201	A3P	N3-C2-N1	-4.60	121.63	128.58
5	B	1101	A3P	N3-C2-N1	-4.59	121.63	128.58
5	B	1101	A3P	O4'-C1'-N9	4.46	116.66	108.09
5	B	2201	A3P	C4-C5-N7	-4.36	105.59	110.58
4	B	2202	ANR	C3-C2-C1	4.29	117.22	112.45
4	B	2202	ANR	C18-C1-C2	-4.28	92.51	108.95
4	A	1102	ANR	C3-C2-C1	4.24	117.17	112.45
4	B	2202	ANR	C11-C12-C13	4.02	132.92	127.28
4	B	2202	ANR	C11-C10-C9	4.00	137.32	126.36
4	B	2202	ANR	C7-C6-C5	-3.88	111.45	122.61
4	B	2202	ANR	C18-C1-C6	3.78	116.17	110.24
4	A	1102	ANR	C11-C10-C9	3.75	136.65	126.36
5	B	1101	A3P	O3'-C3'-C4'	-3.73	96.88	110.03
4	A	1102	ANR	C7-C6-C5	-3.67	112.05	122.61
4	A	1102	ANR	C18-C1-C2	-3.47	95.63	108.95
5	B	1101	A3P	C4-C5-N7	-3.42	106.67	110.58
5	B	2201	A3P	C5-C4-N3	-3.36	122.09	126.72
5	B	2201	A3P	O2'-C2'-C1'	3.34	121.62	110.10
4	A	1102	ANR	C3-C4-C5	3.30	130.30	123.62
4	B	2202	ANR	C3-C4-C5	3.25	130.20	123.62
5	B	1101	A3P	O2'-C2'-C1'	3.17	121.01	110.10
5	B	2201	A3P	O3'-C3'-C4'	-3.15	98.92	110.03
5	B	1101	A3P	C5-C4-N3	-3.08	122.47	126.72
5	B	2201	A3P	N9-C8-N7	-3.02	109.65	113.94
4	A	1102	ANR	C18-C1-C6	3.01	114.96	110.24
4	A	1102	ANR	C11-C12-C13	2.86	131.29	127.28
5	B	2201	A3P	C6-C5-N7	2.71	137.31	132.09
4	B	2202	ANR	C20-C13-C12	-2.64	118.53	122.82
4	A	1102	ANR	C20-C13-C12	-2.53	118.72	122.82
5	B	1101	A3P	O2'-C2'-C3'	2.51	118.22	111.19
5	B	1101	A3P	O3'-C3'-C2'	-2.34	103.27	111.68
5	B	2201	A3P	C2-N3-C4	2.33	117.53	111.83
4	A	1102	ANR	C17-C1-C2	-2.33	99.99	108.95
5	B	2201	A3P	O3'-C3'-C2'	-2.30	103.41	111.68
4	B	2202	ANR	C19-C9-C10	2.25	121.52	118.09
4	A	1102	ANR	C19-C9-C10	2.22	121.47	118.09
5	B	2201	A3P	C5-N7-C8	2.21	106.93	103.45
5	B	2201	A3P	O2'-C2'-C3'	2.16	117.24	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	A3P	N9-C8-N7	-2.16	110.88	113.94
5	B	2201	A3P	C3'-C2'-C1'	2.10	104.51	99.89
5	B	1101	A3P	C5'-C4'-C3'	-2.08	107.43	114.38
5	B	1101	A3P	O3'-P1-O1P	-2.07	101.95	109.33
5	B	1101	A3P	C5-C6-N6	-2.04	118.25	123.29
5	B	1101	A3P	C2'-C1'-N9	2.02	118.31	113.30
5	B	1101	A3P	C2'-C3'-C4'	2.01	106.75	103.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	ANR	C11-C10-C9-C19
4	A	1102	ANR	C11-C10-C9-C8
5	B	1101	A3P	C5'-O5'-P2-O6P
4	A	1102	ANR	C10-C11-C12-C13
4	B	2202	ANR	C11-C10-C9-C19
4	B	2202	ANR	C11-C10-C9-C8
5	B	2201	A3P	C3'-O3'-P1-O2P
4	B	2202	ANR	C10-C11-C12-C13
5	B	2201	A3P	C5'-O5'-P2-O6P
5	B	1101	A3P	C4'-C3'-O3'-P1
5	B	1101	A3P	C3'-O3'-P1-O2P
4	B	2202	ANR	C6-C7-C8-C9

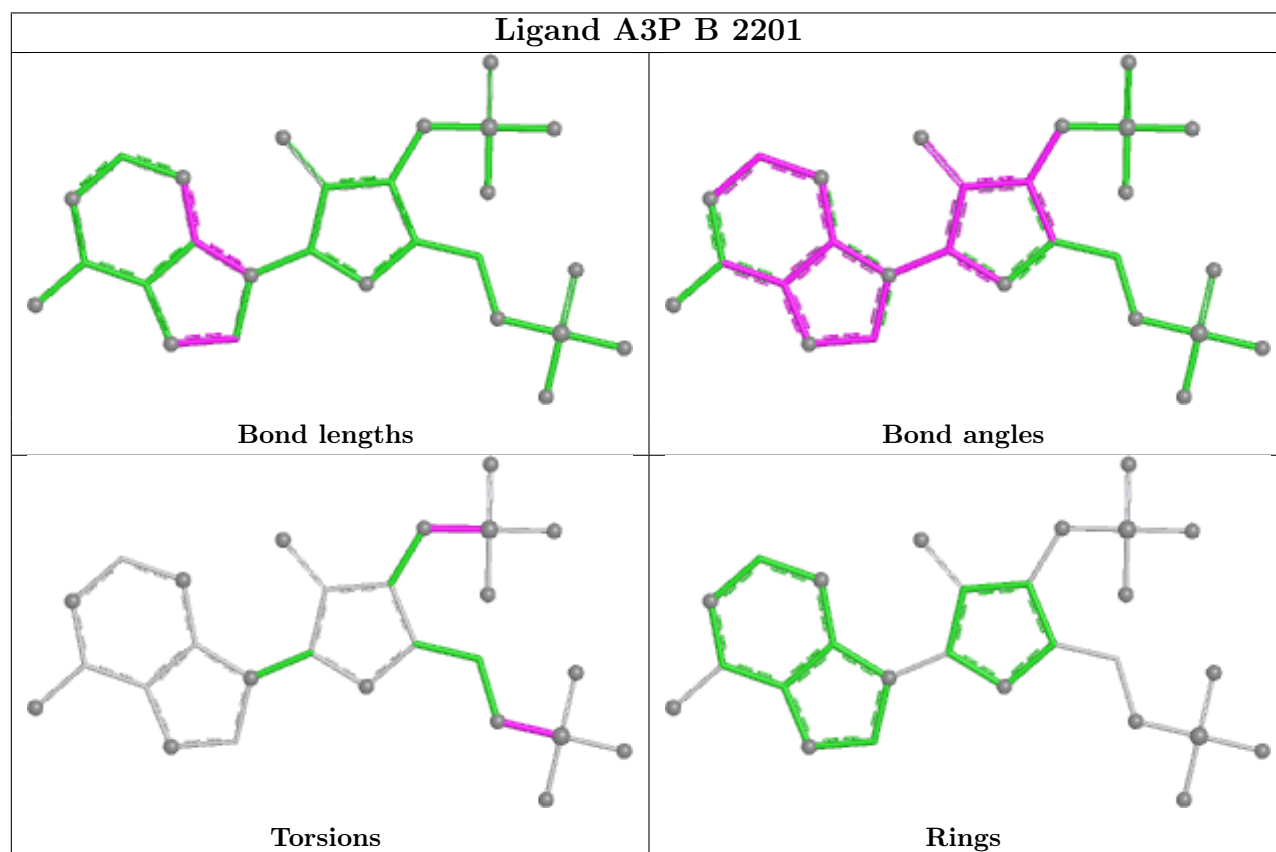
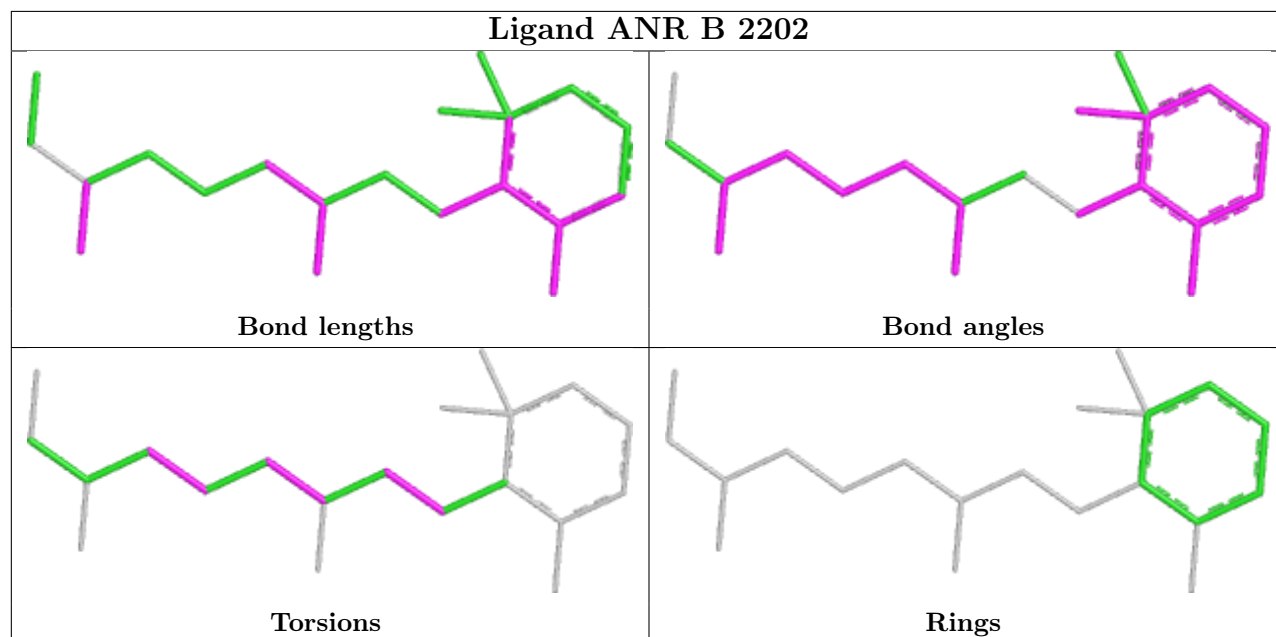
There are no ring outliers.

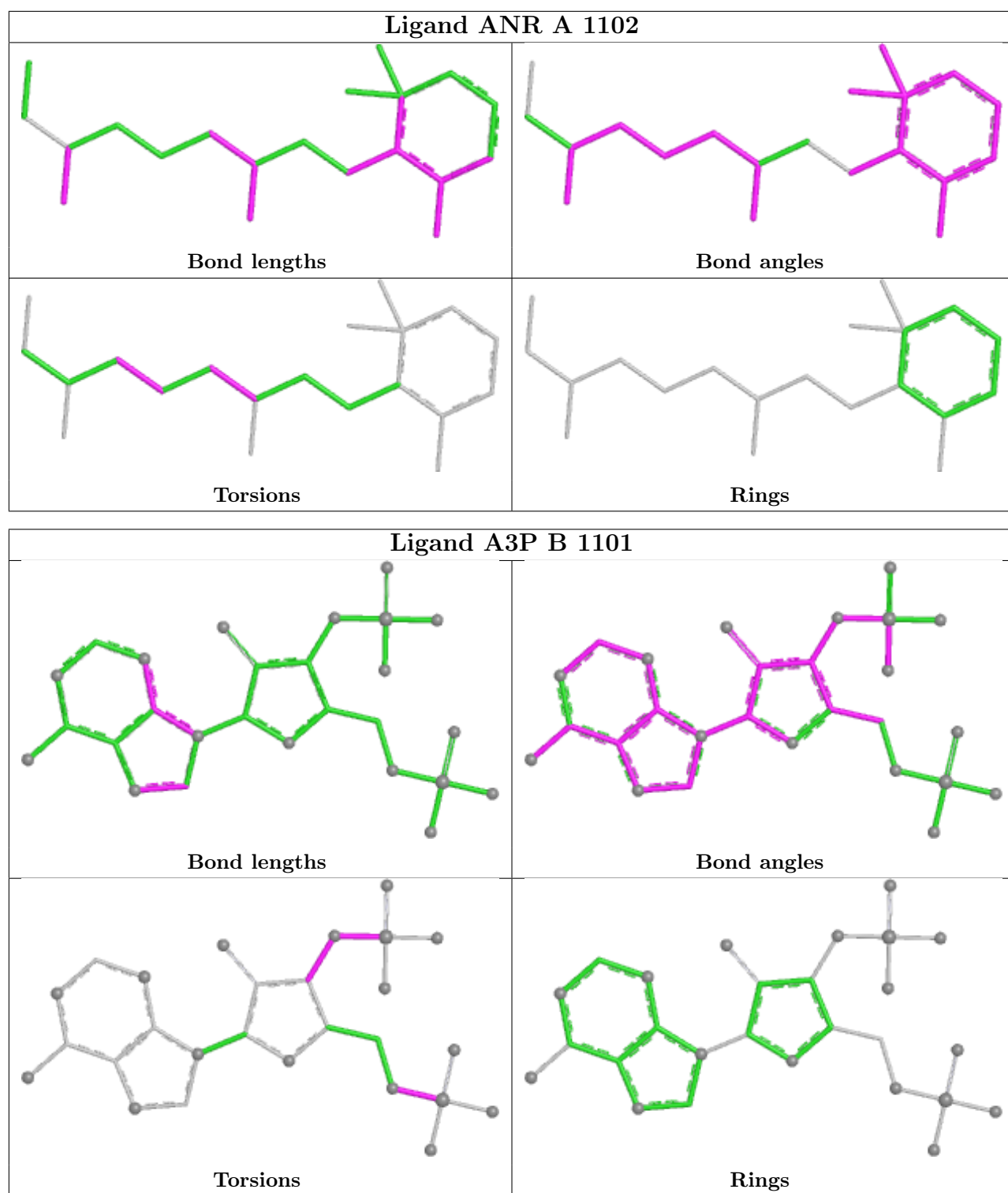
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2202	ANR	1	0
4	A	1102	ANR	2	0
5	B	1101	A3P	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.