



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:35 PM GMT

PDB ID : 1XU7  
Title : Crystal Structure of the Interface Open Conformation of Tetrameric 11b-HSD1  
Authors : Hosfield, D.J.; Wu, Y.; Skene, R.J.; Hilger, M.; Jennings, A.; Snell, G.P.; Aertgeerts, K.  
Deposited on : 2004-10-25  
Resolution : 1.80 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](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

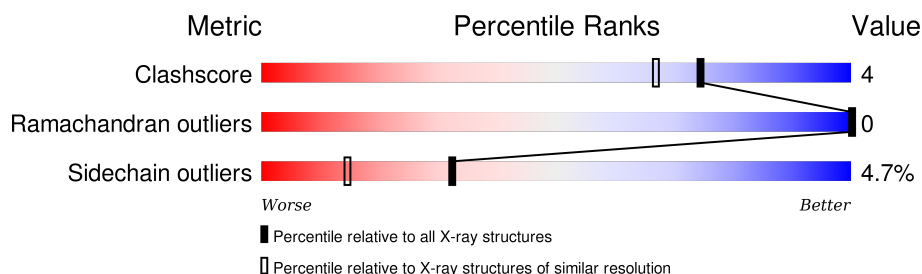
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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	286	 85% 7% 8%
1	B	286	 82% 10% 8%
1	C	286	 79% 12% 8%
1	D	286	 80% 10% 9%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8921 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 Corticosteroid 11-beta-dehydrogenase, isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	10	0
			2014	1284	341	374	15			
1	B	262	Total	C	N	O	S	0	10	0
			2008	1281	340	372	15			
1	C	262	Total	C	N	O	S	0	9	0
			2008	1281	340	372	15			
1	D	261	Total	C	N	O	S	0	10	0
			2001	1277	339	370	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	INitiating methionine	UNP P28845
A	8	LYS	-	cloning artifact	UNP P28845
A	9	HIS	-	cloning artifact	UNP P28845
A	10	GLN	-	cloning artifact	UNP P28845
A	11	HIS	-	cloning artifact	UNP P28845
A	12	GLN	-	cloning artifact	UNP P28845
A	13	HIS	-	cloning artifact	UNP P28845
A	14	GLN	-	cloning artifact	UNP P28845
A	15	HIS	-	cloning artifact	UNP P28845
A	16	GLN	-	cloning artifact	UNP P28845
A	17	HIS	-	cloning artifact	UNP P28845
A	18	GLN	-	cloning artifact	UNP P28845
A	19	HIS	-	cloning artifact	UNP P28845
A	20	GLN	-	cloning artifact	UNP P28845
A	21	GLN	-	cloning artifact	UNP P28845
A	22	PRO	-	cloning artifact	UNP P28845
A	23	LEU	-	cloning artifact	UNP P28845
A	272	SER	CYS	engineered	UNP P28845
B	7	MET	-	INitiating methionine	UNP P28845
B	8	LYS	-	cloning artifact	UNP P28845
B	9	HIS	-	cloning artifact	UNP P28845

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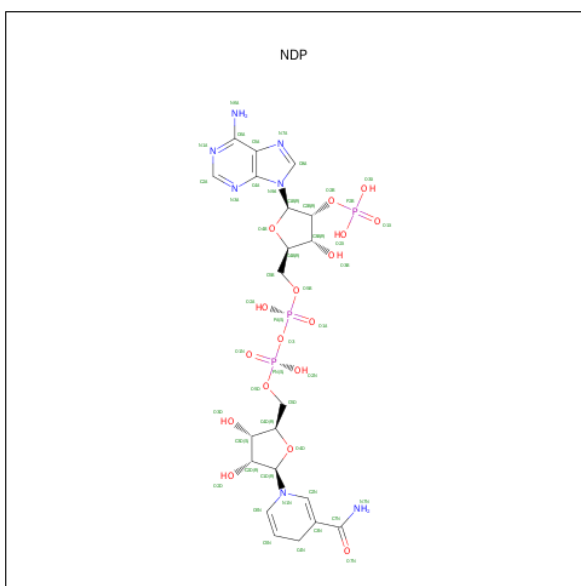
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	cloning artifact	UNP P28845
B	11	HIS	-	cloning artifact	UNP P28845
B	12	GLN	-	cloning artifact	UNP P28845
B	13	HIS	-	cloning artifact	UNP P28845
B	14	GLN	-	cloning artifact	UNP P28845
B	15	HIS	-	cloning artifact	UNP P28845
B	16	GLN	-	cloning artifact	UNP P28845
B	17	HIS	-	cloning artifact	UNP P28845
B	18	GLN	-	cloning artifact	UNP P28845
B	19	HIS	-	cloning artifact	UNP P28845
B	20	GLN	-	cloning artifact	UNP P28845
B	21	GLN	-	cloning artifact	UNP P28845
B	22	PRO	-	cloning artifact	UNP P28845
B	23	LEU	-	cloning artifact	UNP P28845
B	272	SER	CYS	engineered	UNP P28845
C	7	MET	-	INitiating methionine	UNP P28845
C	8	LYS	-	cloning artifact	UNP P28845
C	9	HIS	-	cloning artifact	UNP P28845
C	10	GLN	-	cloning artifact	UNP P28845
C	11	HIS	-	cloning artifact	UNP P28845
C	12	GLN	-	cloning artifact	UNP P28845
C	13	HIS	-	cloning artifact	UNP P28845
C	14	GLN	-	cloning artifact	UNP P28845
C	15	HIS	-	cloning artifact	UNP P28845
C	16	GLN	-	cloning artifact	UNP P28845
C	17	HIS	-	cloning artifact	UNP P28845
C	18	GLN	-	cloning artifact	UNP P28845
C	19	HIS	-	cloning artifact	UNP P28845
C	20	GLN	-	cloning artifact	UNP P28845
C	21	GLN	-	cloning artifact	UNP P28845
C	22	PRO	-	cloning artifact	UNP P28845
C	23	LEU	-	cloning artifact	UNP P28845
C	272	SER	CYS	engineered	UNP P28845
D	7	MET	-	INitiating methionine	UNP P28845
D	8	LYS	-	cloning artifact	UNP P28845
D	9	HIS	-	cloning artifact	UNP P28845
D	10	GLN	-	cloning artifact	UNP P28845
D	11	HIS	-	cloning artifact	UNP P28845
D	12	GLN	-	cloning artifact	UNP P28845
D	13	HIS	-	cloning artifact	UNP P28845
D	14	GLN	-	cloning artifact	UNP P28845
D	15	HIS	-	cloning artifact	UNP P28845

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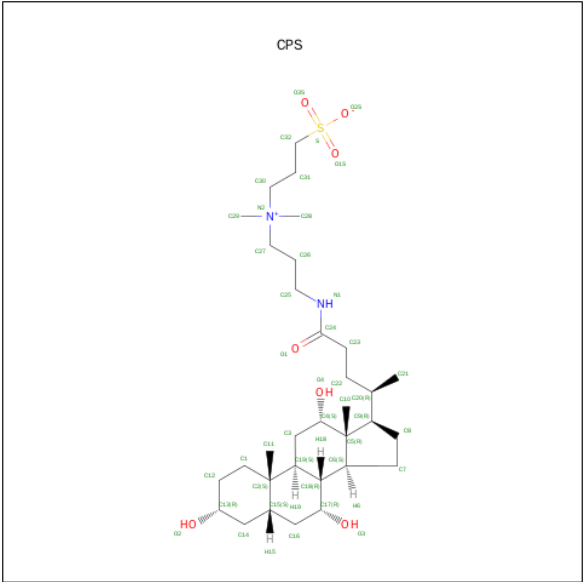
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	cloning artifact	UNP P28845
D	17	HIS	-	cloning artifact	UNP P28845
D	18	GLN	-	cloning artifact	UNP P28845
D	19	HIS	-	cloning artifact	UNP P28845
D	20	GLN	-	cloning artifact	UNP P28845
D	21	GLN	-	cloning artifact	UNP P28845
D	22	PRO	-	cloning artifact	UNP P28845
D	23	LEU	-	cloning artifact	UNP P28845
D	272	SER	CYS	engineered	UNP P28845

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula:  $C_{32}H_{58}N_2O_7S$ ).




Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	B	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	C	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	D	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	A	1	Total	C	O			0	0
			22	19	3				
3	C	1	Total	C	O			0	0
			22	19	3				

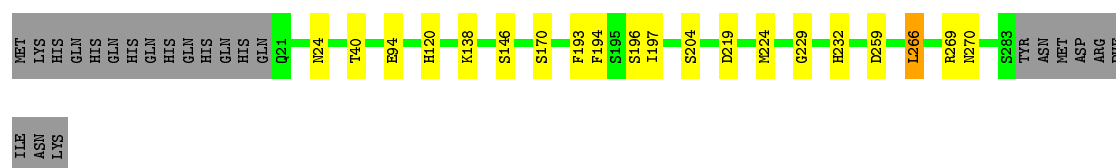
- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	113	Total	O	0	0
			113	113		
4	C	140	Total	O	0	0
			140	140		
4	D	104	Total	O	0	0
			104	104		

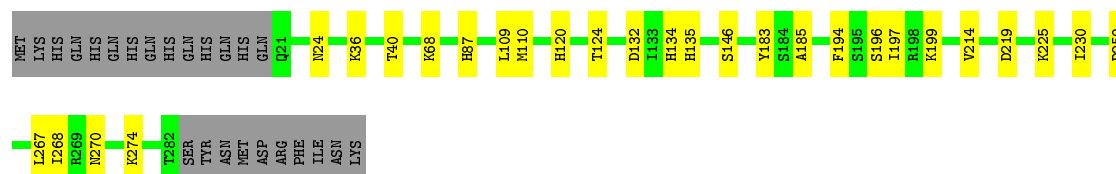


Note EDS was not executed.

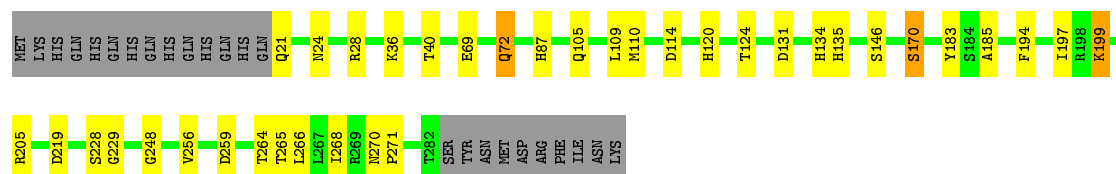
- Chain A:  85% 7% 8%

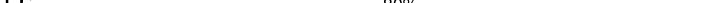


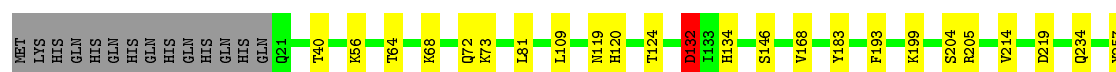
- Chain B:  82% 10% 8%



- Chain C:  79% 12% 8%



- Chain D:  80% 10% 9%



Y258	D259	L262	W263	T264	T268	R269	W270	K274	W275	L276	S281	THR	SER	TYR	ASN	MET	ASP	ARG	PHE	ILE	ASN	LYS
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.43 Å   159.62 Å   73.54 Å 90.00°   93.07°   90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.1 (20.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.197 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: NDP, CPS

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	0.31	0/2048	0.56	2/2766 (0.1%)
1	B	0.31	0/2042	0.58	3/2758 (0.1%)
1	C	0.31	0/2042	0.59	4/2758 (0.1%)
1	D	0.29	0/2035	0.57	3/2748 (0.1%)
All	All	0.31	0/8167	0.57	12/11030 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	219	ASP	CB-CG-OD2	6.16	123.85	118.30
1	D	219	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	219	ASP	CB-CG-OD2	5.95	123.66	118.30
1	B	259	ASP	CB-CG-OD2	5.28	123.05	118.30

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	2014	0	2041	11	0
1	B	2008	0	2036	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2008	0	2038	18	0
1	D	2001	0	2029	12	0
2	A	48	0	26	0	0
2	B	48	0	26	1	0
2	C	48	0	24	4	0
2	D	48	0	24	5	0
3	A	64	0	88	2	0
3	B	42	0	58	3	0
3	C	64	0	88	5	0
3	D	42	0	58	3	0
4	A	129	0	0	2	0
4	B	113	0	0	3	0
4	C	140	0	0	4	0
4	D	104	0	0	1	0
All	All	8921	0	8536	68	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 4.

The worst 5 of 68 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)
2:D:528:NDP:N3A	2:D:528:NDP:C4A	1.73	1.50
2:D:528:NDP:O5B	2:D:528:NDP:C5B	1.64	1.46
2:C:526:NDP:C3B	2:C:526:NDP:O3B	1.64	1.43
1:A:196[A]:SER:HB2	4:B:973:HOH:O	1.80	0.81
1:C:69:GLU:O	1:C:72:GLN:HG3	1.82	0.79

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	261/286 (91%)	252 (97%)	9 (3%)	0	100	100
1	B	260/286 (91%)	249 (96%)	11 (4%)	0	100	100
1	C	260/286 (91%)	250 (96%)	10 (4%)	0	100	100
1	D	259/286 (91%)	249 (96%)	10 (4%)	0	100	100
All	All	1040/1144 (91%)	1000 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	220/243 (90%)	215 (98%)	5 (2%)	58	42
1	B	219/243 (90%)	210 (96%)	9 (4%)	37	19
1	C	219/243 (90%)	208 (95%)	11 (5%)	30	13
1	D	218/243 (90%)	202 (93%)	16 (7%)	17	5
All	All	876/972 (90%)	835 (95%)	41 (5%)	32	14

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	109	LEU
1	C	205	ARG
1	D	268	ILE
1	C	124[A]	THR
1	C	170	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	ASN
1	C	77	HIS
1	D	120	HIS

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Mol	Chain	Res	Type
1	C	24	ASN
1	C	72	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	CPS	A	1	-	25,25,45	0.53	0	37,41,70	1.41	8 (21%)
2	NDP	A	522	-	42,52,52	3.67	18 (42%)	55,80,80	2.52	15 (27%)
3	CPS	A	523	-	44,45,45	1.66	9 (20%)	67,70,70	1.08	5 (7%)
2	NDP	B	524	-	42,52,52	4.02	21 (50%)	55,80,80	2.61	16 (29%)
3	CPS	B	525	-	44,45,45	1.59	10 (22%)	67,70,70	1.23	7 (10%)
3	CPS	C	2	-	25,25,45	0.53	0	37,41,70	1.03	2 (5%)
2	NDP	C	526	-	42,52,52	4.86	22 (52%)	55,80,80	2.48	16 (29%)
3	CPS	C	527	-	44,45,45	1.66	9 (20%)	67,70,70	1.10	5 (7%)
2	NDP	D	528	-	42,52,52	5.79	27 (64%)	55,80,80	2.41	15 (27%)
3	CPS	D	529	-	44,45,45	1.52	10 (22%)	67,70,70	1.07	4 (5%)

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	CPS	A	1	-	-	0/0/61/90	0/4/4/4
2	NDP	A	522	-	-	0/30/77/77	0/5/5/5
3	CPS	A	523	-	-	0/25/90/90	0/4/4/4
2	NDP	B	524	-	-	0/30/77/77	0/5/5/5
3	CPS	B	525	-	-	0/25/90/90	0/4/4/4
3	CPS	C	2	-	-	0/0/61/90	0/4/4/4
2	NDP	C	526	-	-	0/30/77/77	0/5/5/5
3	CPS	C	527	-	-	0/25/90/90	0/4/4/4
2	NDP	D	528	-	-	0/30/77/77	0/5/5/5
3	CPS	D	529	-	-	0/25/90/90	0/4/4/4

The worst 5 of 126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	528	NDP	C3B-C2B	-12.22	1.25	1.53
2	C	526	NDP	C4N-C5N	-10.05	1.27	1.49
2	B	524	NDP	C3B-C2B	-10.00	1.30	1.53
2	A	522	NDP	C3B-C2B	-9.42	1.31	1.53
2	C	526	NDP	C3B-C2B	-9.22	1.32	1.53

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	524	NDP	N3A-C2A-N1A	-13.06	118.89	128.89
2	A	522	NDP	N3A-C2A-N1A	-12.30	119.47	128.89
2	C	526	NDP	N3A-C2A-N1A	-12.30	119.48	128.89
2	D	528	NDP	N3A-C2A-N1A	-11.29	120.25	128.89
2	A	522	NDP	C3N-C2N-N1N	-3.66	117.90	123.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	523	CPS	2	0
2	B	524	NDP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	525	CPS	3	0
3	C	2	CPS	2	0
2	C	526	NDP	4	0
3	C	527	CPS	3	0
2	D	528	NDP	5	0
3	D	529	CPS	3	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 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.