



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:49 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 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

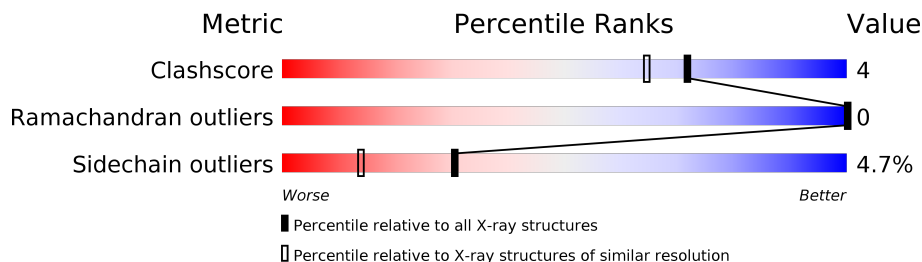
1 Overall quality at a glance

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	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (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 ≥ 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	
1	B	286	
1	C	286	
1	D	286	

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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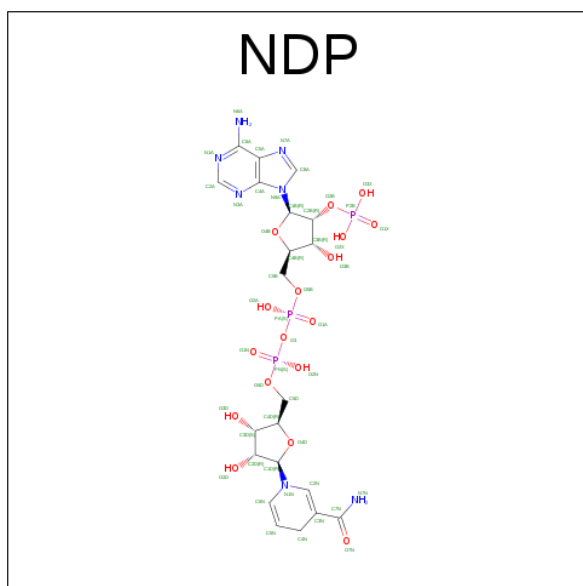
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	cloning artifact	UNP P28845
B	11	HIS	-	cloning artifact	UNP P28845
B	12	GLN	-	cloning artifact	UNP P28845
B	13	HIS	-	cloning artifact	UNP P28845
B	14	GLN	-	cloning artifact	UNP P28845
B	15	HIS	-	cloning artifact	UNP P28845
B	16	GLN	-	cloning 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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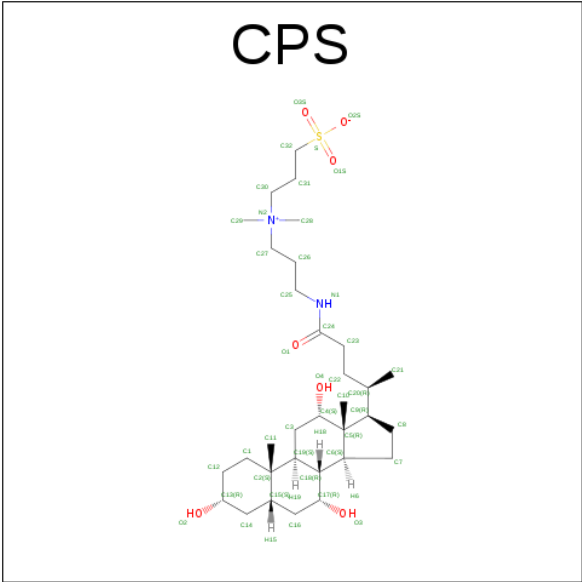
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	cloning artifact	UNP P28845
D	17	HIS	-	cloning artifact	UNP P28845
D	18	GLN	-	cloning artifact	UNP P28845
D	19	HIS	-	cloning artifact	UNP P28845
D	20	GLN	-	cloning artifact	UNP P28845
D	21	GLN	-	cloning artifact	UNP P28845
D	22	PRO	-	cloning 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.

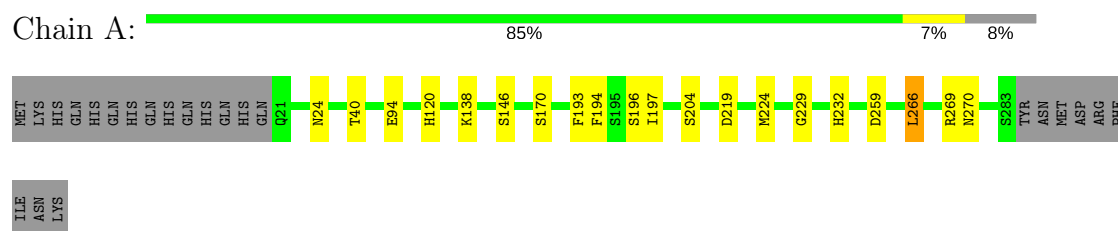
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	113	Total	O	0	0
			113	113		
4	C	140	Total	O	0	0
			140	140		
4	D	104	Total	O	0	0
			104	104		

3 Residue-property plots

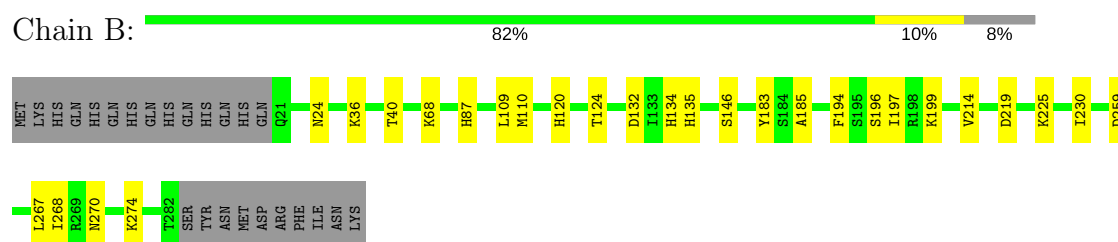
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

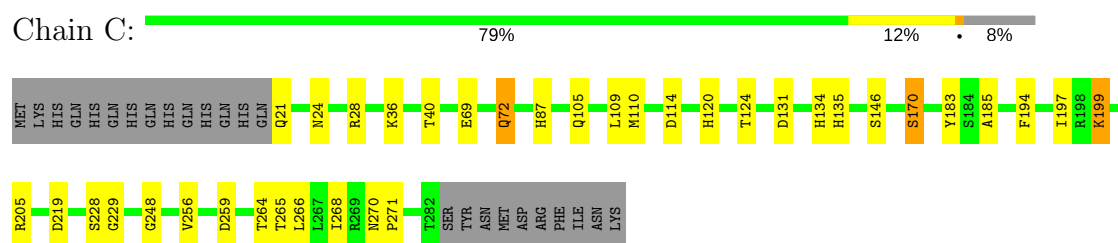
- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1



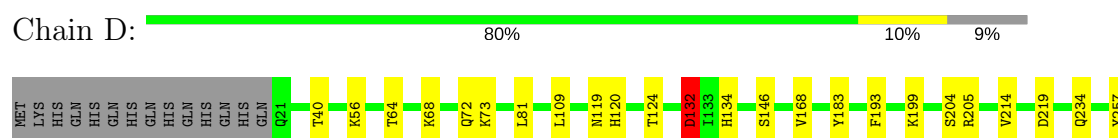
- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1



Y258	D259	L262	K263	L264	L268	K269	N270	K274	L275	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 is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.43Å 159.62Å 73.54Å 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 ²)	17.0	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: 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.

All (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
1	D	132	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	259	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	259	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	259	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	114	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	132	ASP	CB-CG-OD2	5.05	122.84	118.30
1	C	131	ASP	CB-CG-OD2	5.03	122.83	118.30

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

All (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
4:A:961:HOH:O	1:B:196[A]:SER:HB2	1.84	0.78
2:D:528:NDP:C2A	2:D:528:NDP:C4A	2.62	0.77
2:D:528:NDP:C5B	2:D:528:NDP:PA	2.73	0.76
2:C:526:NDP:C2B	2:C:526:NDP:O3B	2.34	0.75
1:A:224:MET:O	1:A:232:HIS:HE1	1.70	0.74
2:C:526:NDP:C4B	2:C:526:NDP:O3B	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:GLN:HG3	4:C:836:HOH:O	1.97	0.63
1:D:132:ASP:HB2	4:D:863:HOH:O	1.98	0.63
1:C:40:THR:OG1	1:C:120:HIS:HD2	1.85	0.58
2:C:526:NDP:C3B	2:C:526:NDP:HO3A	2.08	0.56
1:D:257:TYR:CE2	1:D:268:ILE:HD11	2.43	0.53
1:C:271:PRO:HB2	3:C:2:CPS:H7	1.91	0.53
1:D:120:HIS:HE1	1:D:146:SER:OG	1.92	0.52
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.91	0.52
3:B:525:CPS:H21A	3:B:525:CPS:H4	1.91	0.52
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.91	0.51
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.94	0.50
1:B:194:PHE:HA	1:B:197:ILE:HG12	1.91	0.50
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.94	0.50
1:B:120:HIS:HE1	1:B:146:SER:OG	1.96	0.49
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.96	0.48
1:C:265:THR:HA	1:C:268:ILE:HD12	1.94	0.48
1:C:185:ALA:HB2	1:D:193:PHE:HB2	1.96	0.48
1:C:228:SER:HA	1:C:229:GLY:HA2	1.62	0.47
1:C:248:GLY:HA3	1:C:256:VAL:CG2	2.44	0.47
1:C:120:HIS:HE1	1:C:146:SER:OG	1.96	0.47
1:A:266:LEU:HD23	3:C:2:CPS:H10	1.96	0.47
1:A:120:HIS:HE1	1:A:146:SER:OG	1.97	0.46
1:C:134:HIS:CG	1:C:135:HIS:N	2.83	0.46
1:C:199:LYS:HE2	4:C:800:HOH:O	2.16	0.46
1:A:94:GLU:OE1	1:A:138:LYS:NZ	2.46	0.46
1:A:224:MET:O	1:A:232:HIS:CE1	2.61	0.46
2:D:528:NDP:N3A	2:D:528:NDP:H1B	2.32	0.45
1:B:274:LYS:HA	1:B:274:LYS:HD2	1.81	0.44
3:C:527:CPS:H261	3:C:527:CPS:H29B	1.84	0.44
3:C:527:CPS:H4	3:C:527:CPS:H21A	1.99	0.44
1:A:194:PHE:HA	1:A:197:ILE:HG12	1.99	0.44
1:A:229:GLY:O	1:A:232:HIS:HD2	2.01	0.44
1:D:214:VAL:HG11	1:D:268:ILE:HD13	2.00	0.44
3:B:525:CPS:H29A	3:B:525:CPS:H261	1.65	0.43
1:D:264:THR:O	1:D:268:ILE:HG23	2.18	0.43
1:D:40:THR:HA	1:D:64:THR:HG22	2.01	0.43
1:C:170:SER:HB3	4:C:801:HOH:O	2.18	0.43
1:D:183:TYR:CZ	3:D:529:CPS:H16	2.53	0.43
1:B:214:VAL:HG11	1:B:268:ILE:HG12	2.00	0.43
1:B:134:HIS:CG	1:B:135:HIS:N	2.87	0.43
1:C:36:LYS:HG2	1:C:110:MET:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:NDP:H8A	4:B:642:HOH:O	2.19	0.42
1:A:170:SER:HB3	4:A:546:HOH:O	2.19	0.42
1:B:36:LYS:HG2	1:B:110:MET:HB3	2.02	0.42
1:D:119:ASN:HD22	1:D:168:VAL:HG21	1.85	0.41
1:D:56:LYS:HE2	1:D:81:LEU:HD22	2.01	0.41
3:A:523:CPS:H272	3:A:523:CPS:H31	1.78	0.41
1:B:183:TYR:CZ	3:B:525:CPS:H16	2.55	0.41
1:D:274:LYS:HD2	1:D:274:LYS:HA	1.86	0.41
3:D:529:CPS:H31A	3:D:529:CPS:H271	1.83	0.41
1:C:194:PHE:HA	1:C:197:ILE:HG12	2.02	0.41
1:C:264:THR:O	1:C:268:ILE:HG13	2.20	0.41
3:A:523:CPS:H21A	3:A:523:CPS:H4	2.02	0.41
1:B:87:HIS:HD2	4:B:808:HOH:O	2.04	0.41
1:C:183:TYR:CZ	3:C:527:CPS:H16	2.56	0.40
3:D:529:CPS:H21A	3:D:529:CPS:H4	2.02	0.40
1:C:87:HIS:HD2	4:C:818:HOH:O	2.03	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	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%)	56	41
1	B	219/243 (90%)	210 (96%)	9 (4%)	35	18
1	C	219/243 (90%)	208 (95%)	11 (5%)	28	12
1	D	218/243 (90%)	202 (93%)	16 (7%)	16	5
All	All	876/972 (90%)	835 (95%)	41 (5%)	30	14

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	204[A]	SER
1	A	266	LEU
1	A	269	ARG
1	A	270	ASN
1	B	24	ASN
1	B	68	LYS
1	B	109	LEU
1	B	124[A]	THR
1	B	199	LYS
1	B	225	LYS
1	B	230	ILE
1	B	267	LEU
1	B	270	ASN
1	C	21	GLN
1	C	24	ASN
1	C	28	ARG
1	C	72	GLN
1	C	109	LEU
1	C	124[A]	THR
1	C	170	SER
1	C	199	LYS
1	C	205	ARG
1	C	266	LEU

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Mol	Chain	Res	Type
1	C	270	ASN
1	D	68	LYS
1	D	72	GLN
1	D	73	LYS
1	D	109	LEU
1	D	124[A]	THR
1	D	132	ASP
1	D	134	HIS
1	D	199	LYS
1	D	204[A]	SER
1	D	205	ARG
1	D	234	GLN
1	D	262	LEU
1	D	268	ILE
1	D	270	ASN
1	D	276	LEU
1	D	281	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	232	HIS
1	A	234	GLN
1	A	270	ASN
1	B	77	HIS
1	B	87	HIS
1	B	119	ASN
1	B	120	HIS
1	B	270	ASN
1	C	24	ASN
1	C	72	GLN
1	C	77	HIS
1	C	87	HIS
1	C	119	ASN
1	C	120	HIS
1	C	134	HIS
1	C	270	ASN
1	D	87	HIS
1	D	105	GLN

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Mol	Chain	Res	Type
1	D	119	ASN
1	D	120	HIS
1	D	270	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.55	0	37,41,70	1.45	9 (24%)
2	NDP	A	522	-	43,52,52	3.74	17 (39%)	49,80,80	2.37	12 (24%)
3	CPS	A	523	-	45,45,45	1.90	10 (22%)	68,70,70	1.12	6 (8%)
2	NDP	B	524	-	43,52,52	4.09	21 (48%)	49,80,80	2.46	13 (26%)
3	CPS	B	525	-	45,45,45	1.82	11 (24%)	68,70,70	1.28	8 (11%)
3	CPS	C	2	-	25,25,45	0.55	0	37,41,70	1.07	2 (5%)
2	NDP	C	526	-	43,52,52	4.86	23 (53%)	49,80,80	2.33	13 (26%)
3	CPS	C	527	-	45,45,45	1.97	11 (24%)	68,70,70	1.15	6 (8%)
2	NDP	D	528	-	43,52,52	5.77	27 (62%)	49,80,80	2.30	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CPS	D	529	-	45,45,45	1.82	11 (24%)	68,70,70	1.14	5 (7%)

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

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	528	NDP	C3B-C2B	-12.42	1.25	1.53
2	B	524	NDP	C3B-C2B	-10.16	1.30	1.53
2	C	526	NDP	C4N-C5N	-10.00	1.27	1.49
2	A	522	NDP	C3B-C2B	-9.57	1.31	1.53
2	C	526	NDP	C3B-C2B	-9.37	1.32	1.53
2	D	528	NDP	C4N-C5N	-8.74	1.30	1.49
2	B	524	NDP	C5A-C4A	-8.64	1.21	1.40
2	D	528	NDP	C5A-C4A	-7.57	1.23	1.40
3	C	527	CPS	C32-S	-6.99	1.67	1.77
2	D	528	NDP	P2B-O2X	-6.98	1.26	1.54
3	D	529	CPS	C32-S	-6.70	1.67	1.77
2	B	524	NDP	C4N-C5N	-6.67	1.34	1.49
2	A	522	NDP	C5A-C4A	-6.62	1.25	1.40
3	A	523	CPS	C32-S	-6.02	1.68	1.77
2	A	522	NDP	C4N-C5N	-5.95	1.36	1.49
3	B	525	CPS	C32-S	-5.90	1.68	1.77
2	C	526	NDP	C5A-C4A	-5.60	1.27	1.40
2	D	528	NDP	C1D-N1N	-5.29	1.31	1.46
2	D	528	NDP	C5A-N7A	-5.14	1.22	1.39
2	A	522	NDP	C2D-C3D	-4.95	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	524	NDP	C2D-C3D	-4.87	1.40	1.53
2	D	528	NDP	C2D-C3D	-4.79	1.40	1.53
2	C	526	NDP	C5A-N7A	-4.65	1.23	1.39
2	B	524	NDP	C1D-N1N	-4.62	1.33	1.46
2	A	522	NDP	C5A-N7A	-4.56	1.23	1.39
2	B	524	NDP	PA-O2A	-4.29	1.33	1.55
2	C	526	NDP	P2B-O2X	-4.19	1.37	1.54
2	C	526	NDP	C2A-N3A	-4.04	1.25	1.32
2	C	526	NDP	P2B-O1X	-3.99	1.37	1.50
2	B	524	NDP	C5A-N7A	-3.76	1.26	1.39
2	B	524	NDP	C3D-C4D	-3.36	1.44	1.53
2	A	522	NDP	C3D-C4D	-3.34	1.44	1.53
2	D	528	NDP	O4B-C1B	-3.08	1.37	1.41
2	D	528	NDP	PA-O2A	-3.04	1.39	1.55
2	D	528	NDP	PN-O2N	-3.03	1.39	1.55
2	C	526	NDP	C3B-C4B	-2.87	1.45	1.53
2	C	526	NDP	PA-O1A	-2.87	1.40	1.50
2	D	528	NDP	P2B-O1X	-2.78	1.41	1.50
2	C	526	NDP	C2D-C3D	-2.71	1.46	1.53
2	C	526	NDP	PA-O5B	-2.71	1.47	1.59
2	D	528	NDP	PA-O5B	-2.65	1.47	1.59
3	B	525	CPS	C5-C6	-2.63	1.50	1.55
2	B	524	NDP	P2B-O2X	-2.59	1.44	1.54
3	D	529	CPS	C5-C6	-2.33	1.51	1.55
2	D	528	NDP	C3D-C4D	-2.23	1.47	1.53
2	C	526	NDP	PA-O2A	-2.16	1.44	1.55
2	A	522	NDP	C2D-C1D	-2.09	1.46	1.53
2	A	522	NDP	PN-O2N	-2.09	1.44	1.55
3	C	527	CPS	C8-C9	2.05	1.58	1.54
2	A	522	NDP	O4B-C1B	2.11	1.44	1.41
3	D	529	CPS	C3-C4	2.11	1.57	1.53
3	C	527	CPS	C16-C15	2.11	1.57	1.53
2	B	524	NDP	C2D-C1D	2.14	1.60	1.53
3	B	525	CPS	C2-C15	2.20	1.59	1.55
2	B	524	NDP	C2N-C3N	2.26	1.41	1.34
2	C	526	NDP	C6N-N1N	2.28	1.43	1.37
3	D	529	CPS	C8-C9	2.28	1.59	1.54
3	B	525	CPS	C14-C15	2.28	1.57	1.53
3	B	525	CPS	C16-C15	2.28	1.57	1.53
2	C	526	NDP	C8A-N7A	2.36	1.39	1.34
2	D	528	NDP	C6A-N1A	2.36	1.47	1.37
3	D	529	CPS	C18-C19	2.40	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	529	CPS	C10-C5	2.45	1.58	1.54
2	B	524	NDP	O4D-C4D	2.45	1.50	1.45
3	C	527	CPS	C14-C15	2.48	1.57	1.53
3	A	523	CPS	C14-C15	2.52	1.58	1.53
2	C	526	NDP	C2N-C3N	2.52	1.42	1.34
3	A	523	CPS	C8-C9	2.54	1.59	1.54
2	B	524	NDP	C5B-C4B	2.57	1.59	1.51
3	C	527	CPS	C5-C4	2.61	1.58	1.54
3	B	525	CPS	C5-C4	2.63	1.58	1.54
2	D	528	NDP	O4D-C1D	2.64	1.48	1.42
3	B	525	CPS	C8-C9	2.68	1.60	1.54
3	A	523	CPS	C2-C15	2.73	1.60	1.55
2	C	526	NDP	C6A-C5A	2.77	1.57	1.42
2	C	526	NDP	C5B-C4B	2.77	1.60	1.51
2	D	528	NDP	C6A-N6A	2.86	1.45	1.34
3	C	527	CPS	C2-C15	2.89	1.60	1.55
3	A	523	CPS	C16-C15	2.92	1.58	1.53
3	D	529	CPS	C16-C15	2.94	1.58	1.53
3	D	529	CPS	C16-C17	2.95	1.57	1.52
2	D	528	NDP	C6A-C5A	3.01	1.58	1.42
3	D	529	CPS	C2-C15	3.04	1.60	1.55
3	B	525	CPS	C16-C17	3.08	1.57	1.52
3	A	523	CPS	C18-C19	3.09	1.59	1.53
2	C	526	NDP	O3D-C3D	3.09	1.50	1.43
3	A	523	CPS	C5-C4	3.12	1.59	1.54
3	C	527	CPS	C18-C19	3.14	1.60	1.53
3	D	529	CPS	C3-C19	3.14	1.58	1.53
3	B	525	CPS	C18-C19	3.26	1.60	1.53
2	D	528	NDP	O3D-C3D	3.26	1.50	1.43
2	D	528	NDP	C2D-C1D	3.27	1.63	1.53
3	C	527	CPS	C10-C5	3.29	1.59	1.54
3	A	523	CPS	C16-C17	3.29	1.58	1.52
3	A	523	CPS	C20-C9	3.35	1.60	1.54
3	B	525	CPS	C20-C9	3.43	1.60	1.54
3	D	529	CPS	C20-C9	3.47	1.60	1.54
2	B	524	NDP	C6A-C5A	3.51	1.60	1.42
2	A	522	NDP	C6N-C5N	3.53	1.39	1.33
3	C	527	CPS	C20-C9	3.54	1.60	1.54
3	C	527	CPS	C16-C17	3.62	1.58	1.52
2	A	522	NDP	C6A-C5A	3.62	1.61	1.42
2	B	524	NDP	C6N-C5N	3.66	1.40	1.33
2	A	522	NDP	O4B-C4B	3.72	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	526	NDP	O4D-C4D	3.88	1.53	1.45
2	D	528	NDP	C2N-C3N	3.88	1.46	1.34
3	B	525	CPS	C3-C19	3.99	1.60	1.53
3	A	523	CPS	C3-C19	4.30	1.60	1.53
2	B	524	NDP	O3D-C3D	4.46	1.53	1.43
2	A	522	NDP	C8A-N7A	4.54	1.43	1.34
2	D	528	NDP	P2B-O2B	4.58	1.67	1.59
2	A	522	NDP	O3D-C3D	4.58	1.53	1.43
2	B	524	NDP	O3B-C3B	4.74	1.53	1.43
2	D	528	NDP	O4D-C4D	4.76	1.55	1.45
3	C	527	CPS	C3-C19	4.79	1.61	1.53
2	B	524	NDP	P2B-O2B	4.86	1.68	1.59
2	D	528	NDP	O5B-C5B	4.87	1.64	1.44
2	C	526	NDP	C6N-C5N	5.59	1.43	1.33
2	B	524	NDP	C6N-N1N	5.64	1.53	1.37
2	A	522	NDP	O3B-C3B	6.49	1.57	1.43
2	B	524	NDP	C2A-N3A	6.53	1.43	1.32
2	D	528	NDP	O3B-C3B	6.76	1.58	1.43
2	D	528	NDP	C2A-N1A	6.76	1.46	1.33
2	D	528	NDP	C6N-C5N	7.02	1.46	1.33
2	A	522	NDP	C4A-N3A	9.19	1.49	1.35
2	C	526	NDP	O3B-C3B	9.28	1.64	1.43
2	A	522	NDP	C2A-N3A	10.92	1.50	1.32
2	C	526	NDP	C2A-N1A	11.88	1.56	1.33
2	B	524	NDP	C4A-N3A	13.44	1.55	1.35
2	C	526	NDP	C4A-N3A	18.61	1.63	1.35
2	D	528	NDP	C4A-N3A	26.00	1.73	1.35

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	524	NDP	N3A-C2A-N1A	-11.44	118.89	128.86
2	A	522	NDP	N3A-C2A-N1A	-10.78	119.47	128.86
2	C	526	NDP	N3A-C2A-N1A	-10.77	119.48	128.86
2	D	528	NDP	N3A-C2A-N1A	-9.89	120.25	128.86
2	A	522	NDP	O3B-C3B-C4B	-3.74	100.17	111.09
2	B	524	NDP	O3D-C3D-C4D	-3.73	100.19	111.09
2	A	522	NDP	C3N-C2N-N1N	-3.57	117.90	123.08
2	B	524	NDP	O3B-C3B-C4B	-3.52	100.80	111.09
2	A	522	NDP	C4B-O4B-C1B	-3.44	106.11	109.77
3	D	529	CPS	C9-C5-C4	-3.43	114.52	117.67
2	D	528	NDP	O3D-C3D-C4D	-3.38	101.21	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	525	CPS	C9-C5-C4	-3.38	114.56	117.67
2	C	526	NDP	O3D-C3D-C4D	-3.35	101.30	111.09
2	C	526	NDP	C4B-O4B-C1B	-3.32	106.23	109.77
2	A	522	NDP	O3D-C3D-C4D	-3.32	101.40	111.09
3	C	527	CPS	C9-C5-C4	-3.28	114.66	117.67
2	C	526	NDP	O3B-C3B-C4B	-3.21	101.72	111.09
2	D	528	NDP	C3N-C2N-N1N	-3.14	118.53	123.08
2	B	524	NDP	C3N-C2N-N1N	-3.12	118.56	123.08
2	D	528	NDP	O3B-C3B-C4B	-3.08	102.10	111.09
2	C	526	NDP	C3N-C2N-N1N	-2.93	118.83	123.08
2	D	528	NDP	C4B-O4B-C1B	-2.88	106.71	109.77
3	A	1	CPS	C16-C15-C14	-2.86	107.88	111.13
2	A	522	NDP	O3D-C3D-C2D	-2.86	102.68	111.83
2	C	526	NDP	O3D-C3D-C2D	-2.82	102.79	111.83
2	A	522	NDP	O3B-C3B-C2B	-2.78	103.28	111.18
2	B	524	NDP	O3D-C3D-C2D	-2.74	103.04	111.83
2	D	528	NDP	O3D-C3D-C2D	-2.72	103.13	111.83
2	B	524	NDP	C4B-O4B-C1B	-2.59	107.02	109.77
2	B	524	NDP	O3B-C3B-C2B	-2.47	104.15	111.18
3	A	1	CPS	C19-C18-C17	-2.46	109.04	111.92
2	C	526	NDP	O3B-C3B-C2B	-2.41	104.33	111.18
2	B	524	NDP	C1D-N1N-C6N	-2.29	115.80	120.77
3	A	523	CPS	C9-C5-C4	-2.29	115.57	117.67
2	C	526	NDP	O2B-P2B-O1X	-2.22	100.55	109.26
3	A	1	CPS	C11-C2-C15	-2.19	106.52	110.30
2	D	528	NDP	C1D-N1N-C6N	-2.15	116.11	120.77
3	A	1	CPS	C11-C2-C1	-2.05	104.87	108.24
3	B	525	CPS	C5-C9-C20	-2.01	117.06	119.49
3	A	1	CPS	C10-C5-C6	2.14	115.78	111.73
3	A	523	CPS	O3S-S-C32	2.15	108.64	106.79
3	C	527	CPS	C7-C6-C5	2.19	105.75	103.57
3	C	2	CPS	C10-C5-C6	2.21	115.91	111.73
3	D	529	CPS	C7-C6-C5	2.26	105.82	103.57
3	A	523	CPS	C3-C19-C18	2.27	114.11	110.82
3	A	523	CPS	C7-C6-C5	2.27	105.83	103.57
3	A	1	CPS	C16-C15-C2	2.32	115.19	112.66
2	B	524	NDP	C3B-C2B-C1B	2.33	107.31	102.75
3	A	1	CPS	C1-C2-C15	2.35	111.43	107.79
3	D	529	CPS	C3-C19-C18	2.37	114.25	110.82
3	C	527	CPS	O3S-S-C32	2.38	108.84	106.79
3	A	1	CPS	C14-C15-C2	2.39	115.27	112.66
3	A	1	CPS	C3-C19-C18	2.47	114.41	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	CPS	C3-C19-C18	2.48	114.42	110.82
2	C	526	NDP	C3D-C2D-C1D	2.59	106.39	101.43
2	C	526	NDP	C3B-C2B-C1B	2.61	107.85	102.75
2	B	524	NDP	C3D-C2D-C1D	2.63	106.47	101.43
3	B	525	CPS	O1S-S-C32	2.66	109.08	106.79
3	B	525	CPS	C7-C6-C5	2.67	106.23	103.57
3	B	525	CPS	C3-C19-C18	2.72	114.76	110.82
3	B	525	CPS	C25-N1-C24	2.73	128.09	122.84
3	A	523	CPS	O2S-S-C32	2.79	109.48	106.06
2	A	522	NDP	C3D-C2D-C1D	2.86	106.91	101.43
3	C	527	CPS	C3-C19-C18	2.89	115.01	110.82
3	C	527	CPS	O2S-S-C32	2.91	109.63	106.06
2	C	526	NDP	C2D-C3D-C4D	2.98	108.43	102.62
2	D	528	NDP	C3B-C2B-C1B	3.05	108.71	102.75
2	A	522	NDP	C3B-C2B-C1B	3.11	108.84	102.75
3	B	525	CPS	O2S-S-C32	3.15	109.93	106.06
3	B	525	CPS	O3S-S-C32	3.21	109.55	106.79
2	B	524	NDP	C2B-C3B-C4B	3.28	109.40	101.95
2	D	528	NDP	C3D-C2D-C1D	3.33	107.82	101.43
2	D	528	NDP	C2B-C3B-C4B	3.35	109.57	101.95
3	C	527	CPS	O1S-S-C32	3.37	109.68	106.79
2	A	522	NDP	C2D-C3D-C4D	3.38	109.20	102.62
3	D	529	CPS	O1S-S-C32	3.44	109.75	106.79
2	B	524	NDP	C2D-C3D-C4D	3.44	109.33	102.62
3	D	529	CPS	O2S-S-C32	3.46	110.31	106.06
2	C	526	NDP	C2B-C3B-C4B	3.69	110.34	101.95
2	A	522	NDP	C2B-C3B-C4B	3.71	110.38	101.95
3	A	523	CPS	O1S-S-C32	3.87	110.12	106.79
2	D	528	NDP	C2D-C3D-C4D	4.03	110.46	102.62
2	A	522	NDP	O4D-C1D-N1N	4.24	116.61	108.07
2	C	526	NDP	O4D-C1D-N1N	4.72	117.58	108.07
2	D	528	NDP	O4D-C1D-N1N	4.97	118.09	108.07
2	B	524	NDP	O4D-C1D-N1N	5.60	119.36	108.07

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	524	NDP	1	0
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 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.