



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2016 – 07:52 PM EDT

PDB ID : 5EPO
Title : The three-dimensional structure of Clostridium absonum 7alpha-hydroxysteroid dehydrogenase
Authors : Lou, D.; Wang, B.; Wang, F.
Deposited on : 2015-11-12
Resolution : 2.00 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

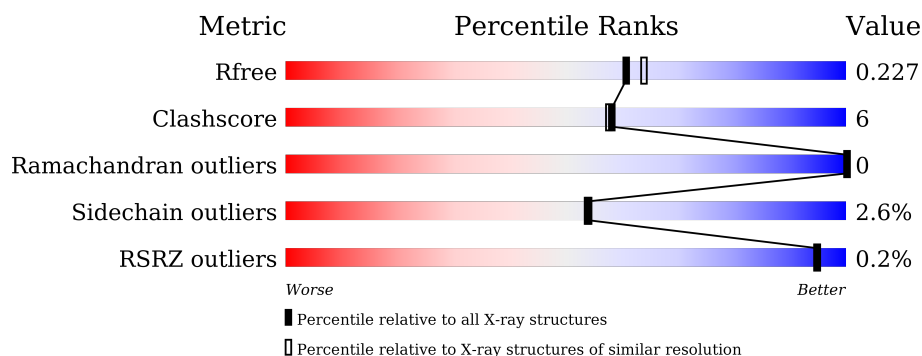
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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.

Mol	Chain	Length	Quality of chain
1	A	262	<div> <div>93%</div> <div>6% .</div> </div>
1	B	262	<div> <div>90%</div> <div>8% .</div> </div>
1	C	262	<div> <div>92%</div> <div>5% ..</div> </div>
1	D	262	<div> <div>94%</div> <div>5%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	B	301	-	-	-	X
3	TUD	A	302	-	-	-	X
3	TUD	B	302	-	-	-	X
3	TUD	D	302	-	-	-	X
4	GOL	D	303	-	-	-	X

2 Entry composition [i](#)

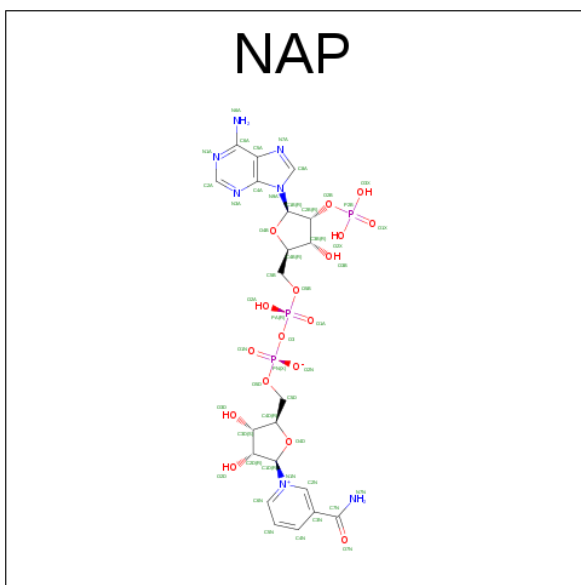
There are 5 unique types of molecules in this entry. The entry contains 9261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 7-alpha-hydroxysteroid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1979	1240	346	386	7			
1	B	261	Total	C	N	O	S	0	0	0
			1979	1240	346	386	7			
1	C	261	Total	C	N	O	S	0	0	0
			1980	1240	346	387	7			
1	D	261	Total	C	N	O	S	0	0	0
			1976	1239	343	386	8			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



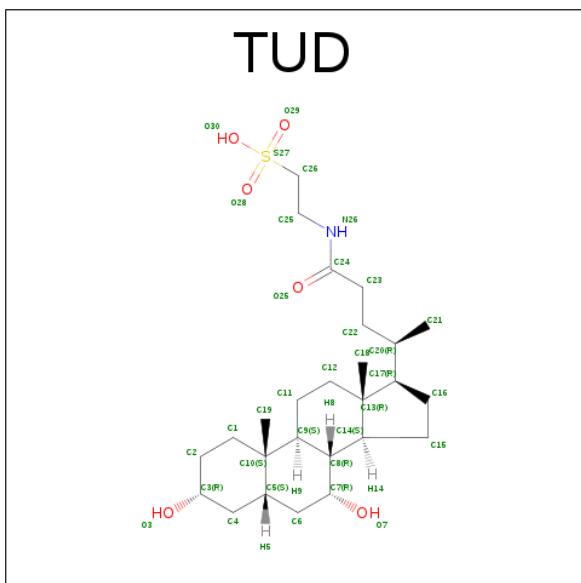
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 TAUROCHENODEOXYCHOLIC ACID (three-letter code: TUD) (formula: $C_{26}H_{45}NO_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			34	26	1	6	1		
3	B	1	Total	C	N	O	S	0	0
			34	26	1	6	1		
3	C	1	Total	C	N	O	S	0	0
			34	26	1	6	1		
3	D	1	Total	C	N	O	S	0	0
			34	26	1	6	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

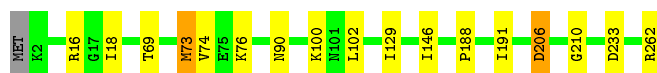
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		
5	B	262	Total	O	0	0
			262	262		
5	C	249	Total	O	0	0
			249	249		
5	D	261	Total	O	0	0
			261	261		

3 Residue-property plots [i](#)

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.

- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain A:  93% 6% .



- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain B:  90% 8% .



- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain C:  92% 5% ..



- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain D:  94% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.18Å 69.68Å 220.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.58 – 2.00 49.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.58-2.00) 98.3 (49.58-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.182 , 0.222 0.189 , 0.227	Depositor DCC
R_{free} test set	3540 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.1	EDS
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 69681 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9261	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: GOL, NAP, TUD

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	0.66	0/2008	0.62	0/2718
1	B	0.68	0/2008	0.67	2/2718 (0.1%)
1	C	0.71	0/2009	0.70	3/2718 (0.1%)
1	D	0.68	0/2005	0.61	0/2714
All	All	0.68	0/8030	0.65	5/10868 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	B	3	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	65	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	2	LYS	N-CA-C	5.33	125.39	111.00
1	C	65	ARG	NE-CZ-NH1	5.28	122.94	120.30

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	1979	0	1980	21	1
1	B	1979	0	1980	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1980	0	1980	18	0
1	D	1976	0	1979	15	0
2	A	48	0	23	14	0
2	B	48	0	24	18	0
2	C	48	0	24	4	0
2	D	48	0	25	13	0
3	A	34	0	45	5	0
3	B	34	0	45	4	0
3	C	34	0	45	2	0
3	D	34	0	45	11	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	223	0	0	2	0
5	B	262	0	0	7	1
5	C	249	0	0	8	3
5	D	261	0	0	5	3
All	All	9261	0	8227	97	4

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 (97) 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:83:ARG:HD3	5:C:566:HOH:O	1.47	1.13
1:B:97:ASN:HB3	5:B:523:HOH:O	1.56	1.04
2:D:301:NAP:C5N	3:D:302:TUD:H162	1.99	0.93
1:C:262:ARG:HD2	5:C:597:HOH:O	1.72	0.89
1:D:1:MET:HE2	1:D:5:GLU:HG2	1.52	0.88
2:C:301:NAP:C4N	3:C:302:TUD:H7	2.04	0.87
1:C:45:GLU:OE2	5:C:401:HOH:O	1.92	0.87
1:B:188:PRO:HB2	2:B:301:NAP:H5N	1.56	0.86
1:B:188:PRO:CB	2:B:301:NAP:H5N	2.06	0.85
1:D:7:LYS:HE3	5:D:518:HOH:O	1.79	0.82
1:A:188:PRO:CB	2:A:301:NAP:H5N	2.10	0.81
1:C:206:ASP:HB3	5:C:533:HOH:O	1.80	0.80
1:A:188:PRO:HB2	2:A:301:NAP:H5N	1.66	0.78
2:D:301:NAP:C3N	3:D:302:TUD:H152	2.16	0.76
1:D:195:ALA:HB3	2:D:301:NAP:H5N	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:NH1	2:B:301:NAP:O2X	2.24	0.71
1:D:195:ALA:CB	2:D:301:NAP:H5N	2.21	0.71
1:A:233:ASP:OD2	5:A:401:HOH:O	2.08	0.70
1:B:188:PRO:HG2	2:B:301:NAP:H6N	1.76	0.66
2:D:301:NAP:C5N	3:D:302:TUD:C16	2.73	0.66
1:B:193:THR:OG1	2:B:301:NAP:N7N	2.29	0.65
1:A:73:MET:HE2	1:A:74:VAL:N	2.12	0.65
1:C:24:GLU:OE2	5:C:402:HOH:O	2.13	0.65
1:B:144:SER:O	1:B:188:PRO:HD2	1.97	0.64
1:C:68:GLU:HB2	5:C:548:HOH:O	1.96	0.64
1:A:188:PRO:HB2	2:A:301:NAP:C5N	2.29	0.63
2:D:301:NAP:C4N	3:D:302:TUD:H152	2.29	0.62
2:D:301:NAP:C6N	3:D:302:TUD:C16	2.78	0.61
1:B:188:PRO:HB2	2:B:301:NAP:C5N	2.30	0.60
1:C:65:ARG:NH2	1:C:91:TYR:OH	2.34	0.60
2:A:301:NAP:H2N	3:A:302:TUD:C15	2.32	0.60
1:D:1:MET:HE2	1:D:5:GLU:CG	2.29	0.60
2:B:301:NAP:C2N	3:B:302:TUD:C15	2.79	0.60
1:B:71:THR:HG23	5:B:466:HOH:O	2.02	0.59
1:A:102:LEU:HD23	1:C:129:ILE:HD12	1.83	0.59
2:A:301:NAP:C2N	3:A:302:TUD:C15	2.81	0.57
1:D:195:ALA:HB3	2:D:301:NAP:C5N	2.34	0.57
1:B:71:THR:HG22	5:B:471:HOH:O	2.03	0.57
1:A:191:ILE:HG12	2:A:301:NAP:H4N	1.87	0.56
1:A:191:ILE:CG1	2:A:301:NAP:H4N	2.36	0.55
2:B:301:NAP:C2N	3:B:302:TUD:H152	2.37	0.55
1:C:188:PRO:HB2	2:C:301:NAP:C5N	2.37	0.54
1:C:2:LYS:NZ	1:C:2:LYS:HB3	2.23	0.53
1:A:18:ILE:CD1	2:A:301:NAP:C5N	2.86	0.53
2:B:301:NAP:H4N	5:B:401:HOH:O	2.02	0.53
2:D:301:NAP:H71N	3:D:302:TUD:H7	1.74	0.53
1:D:94:THR:O	3:D:302:TUD:H261	2.09	0.52
3:A:302:TUD:H121	3:A:302:TUD:H212	1.91	0.52
1:A:73:MET:HE2	1:A:73:MET:C	2.30	0.51
3:D:302:TUD:H121	3:D:302:TUD:H212	1.92	0.51
2:A:301:NAP:C2N	3:A:302:TUD:H152	2.41	0.51
1:C:189:GLY:O	2:C:301:NAP:H4N	2.11	0.51
1:A:18:ILE:HD11	2:A:301:NAP:C5N	2.41	0.50
2:A:301:NAP:C2N	3:A:302:TUD:H151	2.42	0.49
1:B:258:GLU:OE2	5:B:402:HOH:O	2.20	0.49
2:D:301:NAP:C6N	3:D:302:TUD:H162	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:HG23	1:B:83:ARG:HD2	1.94	0.49
1:A:188:PRO:HG2	2:A:301:NAP:H6N	1.94	0.49
1:C:145:THR:HA	1:C:188:PRO:HD2	1.94	0.49
1:B:18:ILE:HD11	2:B:301:NAP:C5N	2.42	0.48
1:B:18:ILE:CD1	2:B:301:NAP:C5N	2.91	0.48
1:C:2:LYS:NZ	1:C:2:LYS:CB	2.76	0.48
1:B:262:ARG:NH2	5:B:412:HOH:O	2.45	0.48
1:C:49:ASP:HB2	5:C:408:HOH:O	2.13	0.48
3:C:302:TUD:H121	3:C:302:TUD:H212	1.94	0.48
1:D:65:ARG:HG2	5:D:573:HOH:O	2.12	0.48
1:B:69:THR:O	1:B:73:MET:HB3	2.14	0.48
1:A:102:LEU:HD23	1:C:129:ILE:CD1	2.44	0.47
1:B:102:LEU:HD12	1:D:122:TYR:CE2	2.50	0.47
1:B:188:PRO:HG2	2:B:301:NAP:C6N	2.41	0.46
1:A:69:THR:O	1:A:73:MET:HG2	2.15	0.46
1:B:129:ILE:HD12	1:D:102:LEU:HD23	1.97	0.46
1:D:2:LYS:HG2	5:D:535:HOH:O	2.15	0.46
1:B:191:ILE:HG12	2:B:301:NAP:H4N	1.97	0.46
1:B:90:ASN:O	2:B:301:NAP:H4D	2.15	0.46
2:D:301:NAP:C6N	2:D:301:NAP:O5D	2.64	0.46
2:B:301:NAP:H2N	3:B:302:TUD:C15	2.46	0.45
1:D:1:MET:CE	1:D:5:GLU:HG2	2.37	0.45
1:A:210:GLY:HA2	1:A:262:ARG:HD3	1.99	0.45
1:A:129:ILE:HD12	1:C:102:LEU:HD23	1.98	0.45
2:B:301:NAP:C2N	3:B:302:TUD:H151	2.47	0.45
2:D:301:NAP:C2N	3:D:302:TUD:H152	2.47	0.45
1:B:83:ARG:HD3	1:B:85:ASP:OD2	2.17	0.44
1:C:100:LYS:O	1:C:156:ILE:HG22	2.17	0.44
1:A:76:LYS:HE2	5:A:424:HOH:O	2.16	0.44
1:A:146:ILE:HA	1:A:146:ILE:HD12	1.92	0.44
1:C:2:LYS:HZ3	1:C:2:LYS:HB3	1.82	0.44
1:B:102:LEU:HD23	1:D:129:ILE:HD12	2.00	0.43
1:A:90:ASN:O	2:A:301:NAP:H4D	2.18	0.43
1:D:7:LYS:CE	5:D:518:HOH:O	2.53	0.42
1:A:188:PRO:CG	2:A:301:NAP:H5N	2.49	0.42
2:D:301:NAP:C2N	3:D:302:TUD:C15	2.97	0.42
1:A:206:ASP:OD2	1:A:262:ARG:NH1	2.52	0.42
2:C:301:NAP:H8A	5:C:547:HOH:O	2.19	0.42
1:B:16:ARG:HG2	2:B:301:NAP:H3B	2.01	0.41
1:D:233:ASP:OD1	5:D:401:HOH:O	2.22	0.41
2:B:301:NAP:C4N	5:B:401:HOH:O	2.52	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:C	5:B:410:HOH:O[4_455]	1.56	0.64
5:C:499:HOH:O	5:D:534:HOH:O[1_565]	2.04	0.16
5:C:403:HOH:O	5:D:445:HOH:O[1_565]	2.05	0.15
5:C:625:HOH:O	5:D:567:HOH:O[1_565]	2.17	0.03

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	259/262 (99%)	252 (97%)	7 (3%)	0	100	100
1	B	259/262 (99%)	256 (99%)	3 (1%)	0	100	100
1	C	259/262 (99%)	254 (98%)	5 (2%)	0	100	100
1	D	259/262 (99%)	253 (98%)	6 (2%)	0	100	100
All	All	1036/1048 (99%)	1015 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	208/209 (100%)	204 (98%)	4 (2%)	65	67
1	B	208/209 (100%)	200 (96%)	8 (4%)	40	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	208/209 (100%)	201 (97%)	7 (3%)	44	41
1	D	208/209 (100%)	205 (99%)	3 (1%)	74	77
All	All	832/836 (100%)	810 (97%)	22 (3%)	54	54

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	73	MET
1	A	100	LYS
1	A	206	ASP
1	B	2	LYS
1	B	16	ARG
1	B	32	LEU
1	B	51	LYS
1	B	73	MET
1	B	112	ARG
1	B	209	LEU
1	B	262	ARG
1	C	2	LYS
1	C	7	LYS
1	C	49	ASP
1	C	65	ARG
1	C	68	GLU
1	C	73	MET
1	C	262	ARG
1	D	50	ILE
1	D	73	MET
1	D	112	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

12 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$
2	NAP	A	301	-	45,52,52	4.33	16 (35%)	55,80,80	2.53	11 (20%)
3	TUD	A	302	-	37,37,37	1.87	4 (10%)	58,58,58	2.48	12 (20%)
4	GOL	A	303	-	5,5,5	0.51	0	5,5,5	0.57	0
2	NAP	B	301	-	45,52,52	4.22	17 (37%)	55,80,80	2.43	11 (20%)
3	TUD	B	302	-	37,37,37	1.85	3 (8%)	58,58,58	1.87	13 (22%)
4	GOL	B	303	-	5,5,5	0.44	0	5,5,5	0.43	0
2	NAP	C	301	-	45,52,52	4.11	14 (31%)	55,80,80	2.17	6 (10%)
3	TUD	C	302	-	37,37,37	1.77	6 (16%)	58,58,58	3.03	12 (20%)
4	GOL	C	303	-	5,5,5	0.43	0	5,5,5	0.34	0
2	NAP	D	301	-	45,52,52	4.18	18 (40%)	55,80,80	2.28	9 (16%)
3	TUD	D	302	-	37,37,37	1.61	3 (8%)	58,58,58	2.26	11 (18%)
4	GOL	D	303	-	5,5,5	0.50	0	5,5,5	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
2	NAP	A	301	-	-	0/27/67/67	0/5/5/5
3	TUD	A	302	-	-	0/16/77/77	0/4/4/4
4	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	NAP	B	301	-	-	0/27/67/67	0/5/5/5
3	TUD	B	302	-	-	0/16/77/77	0/4/4/4
4	GOL	B	303	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	301	-	-	0/27/67/67	0/5/5/5
3	TUD	C	302	-	-	0/16/77/77	0/4/4/4
4	GOL	C	303	-	-	0/4/4/4	0/0/0/0
2	NAP	D	301	-	-	0/27/67/67	0/5/5/5
3	TUD	D	302	-	-	0/16/77/77	0/4/4/4
4	GOL	D	303	-	-	0/4/4/4	0/0/0/0

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	C2D-C1D	-15.07	1.29	1.53
2	B	301	NAP	C2D-C1D	-14.29	1.30	1.53
2	D	301	NAP	C2D-C1D	-14.20	1.31	1.53
2	C	301	NAP	C2D-C1D	-13.85	1.31	1.53
2	A	301	NAP	C2B-C1B	-7.96	1.31	1.53
3	A	302	TUD	C26-S27	-7.94	1.65	1.77
2	C	301	NAP	C2B-C1B	-7.82	1.31	1.53
3	B	302	TUD	C26-S27	-7.80	1.65	1.77
2	D	301	NAP	C2B-C1B	-7.60	1.32	1.53
2	B	301	NAP	C2B-C1B	-7.50	1.32	1.53
3	C	302	TUD	C26-S27	-7.04	1.66	1.77
3	D	302	TUD	C26-S27	-6.30	1.68	1.77
2	B	301	NAP	O4D-C4D	-6.28	1.30	1.45
2	D	301	NAP	O4B-C4B	-6.17	1.30	1.45
2	C	301	NAP	O4D-C4D	-6.07	1.31	1.45
2	A	301	NAP	O4B-C4B	-5.95	1.31	1.45
2	A	301	NAP	O4D-C4D	-5.84	1.31	1.45
2	B	301	NAP	O4B-C4B	-5.52	1.32	1.45
2	C	301	NAP	O4B-C4B	-5.48	1.32	1.45
2	D	301	NAP	O4D-C4D	-5.42	1.32	1.45
2	A	301	NAP	C4N-C3N	-3.66	1.33	1.39
2	B	301	NAP	C4N-C3N	-3.45	1.33	1.39
2	C	301	NAP	O3B-C3B	-3.21	1.35	1.43
3	B	302	TUD	O25-C24	-3.18	1.16	1.23
3	A	302	TUD	O25-C24	-3.03	1.16	1.23
3	D	302	TUD	O25-C24	-2.84	1.17	1.23
2	A	301	NAP	O3B-C3B	-2.79	1.36	1.43
2	D	301	NAP	PN-O2N	-2.61	1.44	1.55
2	B	301	NAP	O3B-C3B	-2.46	1.37	1.43
2	D	301	NAP	O3B-C3B	-2.42	1.37	1.43
3	A	302	TUD	C12-C13	-2.36	1.49	1.54
3	C	302	TUD	C19-C10	-2.34	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	TUD	O25-C24	-2.23	1.18	1.23
3	C	302	TUD	O7-C7	-2.19	1.38	1.43
2	D	301	NAP	P2B-O2X	-2.17	1.47	1.54
2	D	301	NAP	PN-O1N	-2.12	1.43	1.51
2	B	301	NAP	C5N-C4N	-2.09	1.34	1.38
2	C	301	NAP	PN-O2N	-2.08	1.46	1.55
2	C	301	NAP	PN-O1N	-2.00	1.44	1.51
2	A	301	NAP	O7N-C7N	2.03	1.28	1.24
2	B	301	NAP	C2A-N1A	2.03	1.37	1.33
2	A	301	NAP	O2B-C2B	2.10	1.50	1.44
2	B	301	NAP	O7N-C7N	2.11	1.28	1.24
2	B	301	NAP	C2N-C3N	2.13	1.42	1.39
2	D	301	NAP	C2A-N1A	2.14	1.38	1.33
2	D	301	NAP	C2A-N3A	2.18	1.36	1.32
2	D	301	NAP	O2B-C2B	2.26	1.51	1.44
2	D	301	NAP	C5D-C4D	2.28	1.59	1.51
2	C	301	NAP	C2A-N1A	2.28	1.38	1.33
2	B	301	NAP	C3N-C7N	2.33	1.54	1.50
2	A	301	NAP	C2N-C3N	2.34	1.42	1.39
2	B	301	NAP	P2B-O1X	2.40	1.58	1.50
2	D	301	NAP	O2D-C2D	2.40	1.48	1.43
3	C	302	TUD	C8-C7	2.46	1.57	1.53
2	D	301	NAP	C3N-C7N	2.63	1.54	1.50
2	A	301	NAP	C2N-N1N	2.80	1.39	1.35
2	A	301	NAP	C2A-N1A	2.98	1.39	1.33
2	C	301	NAP	O2D-C2D	3.04	1.50	1.43
2	A	301	NAP	C3N-C7N	3.06	1.55	1.50
2	D	301	NAP	C2N-N1N	3.10	1.39	1.35
2	B	301	NAP	C2N-N1N	3.22	1.39	1.35
2	A	301	NAP	O2D-C2D	3.38	1.50	1.43
3	D	302	TUD	O30-S27	3.72	1.60	1.47
2	C	301	NAP	C3N-C7N	3.76	1.56	1.50
2	B	301	NAP	O2D-C2D	3.85	1.52	1.43
2	C	301	NAP	C2N-N1N	4.25	1.41	1.35
2	B	301	NAP	C7N-N7N	4.51	1.42	1.33
3	C	302	TUD	O30-S27	4.76	1.63	1.47
3	B	302	TUD	O30-S27	4.79	1.63	1.47
3	A	302	TUD	O30-S27	4.98	1.64	1.47
2	A	301	NAP	C7N-N7N	5.30	1.43	1.33
2	C	301	NAP	C7N-N7N	5.30	1.43	1.33
2	D	301	NAP	C7N-N7N	5.38	1.43	1.33
2	C	301	NAP	O4B-C1B	11.64	1.57	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	O4B-C1B	12.73	1.59	1.41
2	A	301	NAP	O4B-C1B	12.76	1.59	1.41
2	D	301	NAP	O4D-C1D	13.09	1.59	1.41
2	D	301	NAP	O4B-C1B	13.13	1.60	1.41
2	C	301	NAP	O4D-C1D	13.18	1.60	1.41
2	A	301	NAP	O4D-C1D	13.34	1.60	1.41
2	B	301	NAP	O4D-C1D	13.67	1.60	1.41

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	N3A-C2A-N1A	-12.26	119.24	128.87
2	B	301	NAP	N3A-C2A-N1A	-11.96	119.48	128.87
2	A	301	NAP	N3A-C2A-N1A	-11.51	119.83	128.87
2	C	301	NAP	N3A-C2A-N1A	-11.29	120.00	128.87
3	C	302	TUD	O29-S27-C26	-8.49	100.87	106.87
2	A	301	NAP	O4D-C1D-N1N	-8.35	99.08	108.10
2	C	301	NAP	C1B-N9A-C4A	-6.07	120.03	126.81
2	A	301	NAP	N6A-C6A-N1A	-5.73	108.91	118.52
2	C	301	NAP	N6A-C6A-N1A	-5.65	109.03	118.52
2	B	301	NAP	N6A-C6A-N1A	-5.38	109.49	118.52
2	B	301	NAP	C1B-N9A-C4A	-5.27	120.92	126.81
2	A	301	NAP	C1B-N9A-C4A	-5.26	120.93	126.81
2	D	301	NAP	N6A-C6A-N1A	-5.24	109.72	118.52
2	D	301	NAP	C1B-N9A-C4A	-4.81	121.43	126.81
2	B	301	NAP	O4D-C1D-N1N	-4.63	103.11	108.10
2	B	301	NAP	C4N-C3N-C7N	-3.63	111.48	121.11
3	D	302	TUD	C5-C4-C3	-3.61	107.53	112.88
3	D	302	TUD	C6-C5-C4	-3.50	107.31	111.07
3	C	302	TUD	C19-C10-C9	-3.49	106.58	111.20
3	A	302	TUD	C21-C20-C22	-3.43	104.76	110.33
3	C	302	TUD	C6-C5-C4	-3.42	107.40	111.07
2	B	301	NAP	O7N-C7N-C3N	-3.32	115.91	119.60
3	A	302	TUD	C5-C6-C7	-3.26	110.73	114.44
2	A	301	NAP	C4N-C3N-C7N	-3.15	112.74	121.11
3	A	302	TUD	O30-S27-C26	-2.90	98.96	104.99
3	D	302	TUD	C15-C14-C8	-2.86	114.11	118.34
3	B	302	TUD	C6-C5-C4	-2.81	108.05	111.07
3	B	302	TUD	O29-S27-O28	-2.73	106.25	113.96
3	B	302	TUD	O30-S27-O29	-2.67	105.35	111.26
3	C	302	TUD	C23-C22-C20	-2.53	109.76	114.46
2	D	301	NAP	C4N-C3N-C7N	-2.51	114.45	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	TUD	C18-C13-C17	-2.48	107.05	111.76
2	D	301	NAP	O7N-C7N-C3N	-2.46	116.86	119.60
3	D	302	TUD	O30-S27-C26	-2.38	100.04	104.99
2	A	301	NAP	O7N-C7N-C3N	-2.36	116.98	119.60
2	C	301	NAP	O7N-C7N-N7N	-2.30	119.30	122.58
3	C	302	TUD	O29-S27-O28	-2.20	107.73	113.96
2	D	301	NAP	C4B-O4B-C1B	-2.16	107.35	109.64
2	C	301	NAP	C4B-O4B-C1B	-2.15	107.37	109.64
3	B	302	TUD	C23-C24-N26	-2.13	112.75	116.46
3	A	302	TUD	C15-C14-C13	-2.12	101.34	103.83
2	A	301	NAP	C4B-O4B-C1B	-2.10	107.41	109.64
3	B	302	TUD	C21-C20-C22	-2.10	106.92	110.33
2	B	301	NAP	C4B-O4B-C1B	-2.05	107.47	109.64
3	A	302	TUD	C23-C22-C20	-2.02	110.70	114.46
3	A	302	TUD	C5-C4-C3	-2.00	109.91	112.88
3	B	302	TUD	C4-C3-C2	2.03	113.13	110.53
2	A	301	NAP	O2A-PA-O3	2.05	114.05	105.27
3	A	302	TUD	C2-C1-C10	2.05	116.49	112.81
2	D	301	NAP	C2N-C3N-C4N	2.06	120.60	118.27
3	B	302	TUD	C6-C7-C8	2.08	113.67	111.46
2	B	301	NAP	C2N-C3N-C4N	2.10	120.65	118.27
3	B	302	TUD	C6-C5-C10	2.12	114.93	112.66
2	D	301	NAP	C2D-C3D-C4D	2.19	107.12	102.64
3	C	302	TUD	O3-C3-C2	2.24	115.46	110.04
3	C	302	TUD	C6-C7-C8	2.31	113.91	111.46
3	C	302	TUD	C14-C8-C7	2.33	115.10	111.77
3	B	302	TUD	O30-S27-C26	2.34	109.86	104.99
3	D	302	TUD	C25-N26-C24	2.37	127.49	122.79
3	C	302	TUD	C6-C5-C10	2.37	115.20	112.66
3	D	302	TUD	C12-C13-C17	2.43	120.15	116.58
3	A	302	TUD	C1-C2-C3	2.44	113.66	110.41
3	D	302	TUD	C4-C5-C10	2.45	115.28	112.66
2	B	301	NAP	C3N-C7N-N7N	2.48	120.62	117.82
3	D	302	TUD	C25-C26-S27	2.49	121.08	113.66
3	A	302	TUD	O3-C3-C2	2.50	116.07	110.04
2	A	301	NAP	C3N-C7N-N7N	2.52	120.67	117.82
3	B	302	TUD	O25-C24-C23	2.61	126.50	121.97
3	D	302	TUD	C6-C7-C8	2.69	114.31	111.46
3	B	302	TUD	C1-C10-C5	2.77	110.81	107.76
2	A	301	NAP	C2N-C3N-C7N	2.96	127.75	119.24
2	B	301	NAP	C2N-C3N-C7N	2.98	127.79	119.24
3	A	302	TUD	C9-C8-C7	3.03	115.55	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C2D-C1D-N1N	3.19	119.78	113.53
2	A	301	NAP	C2D-C1D-N1N	3.59	120.56	113.53
3	A	302	TUD	C6-C7-C8	3.65	115.33	111.46
2	C	301	NAP	C3N-C7N-N7N	3.67	121.97	117.82
3	D	302	TUD	C9-C8-C7	3.84	116.53	111.89
3	C	302	TUD	C9-C8-C7	3.86	116.55	111.89
2	D	301	NAP	C3N-C7N-N7N	4.01	122.36	117.82
3	B	302	TUD	O29-S27-C26	6.13	111.20	106.87
3	B	302	TUD	O28-S27-C26	7.42	112.11	106.87
3	D	302	TUD	O29-S27-C26	12.95	116.02	106.87
3	A	302	TUD	O29-S27-C26	15.18	117.60	106.87
3	C	302	TUD	O28-S27-C26	18.50	119.94	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	14	0
3	A	302	TUD	5	0
2	B	301	NAP	18	0
3	B	302	TUD	4	0
2	C	301	NAP	4	0
3	C	302	TUD	2	0
2	D	301	NAP	13	0
3	D	302	TUD	11	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	261/262 (99%)	-0.04	0	100 100	5, 12, 31, 50	0
1	B	261/262 (99%)	-0.25	0	100 100	5, 10, 25, 46	0
1	C	261/262 (99%)	-0.12	1 (0%)	93 93	5, 11, 28, 48	0
1	D	261/262 (99%)	-0.11	1 (0%)	93 93	5, 12, 31, 41	0
All	All	1044/1048 (99%)	-0.13	2 (0%)	95 95	5, 11, 29, 50	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	PRO	2.3
1	C	262	ARG	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	D	303	6/6	0.86	0.21	4.07	21,22,25,34	0
2	NAP	B	301	48/48	0.86	0.23	3.35	23,33,75,86	0
3	TUD	A	302	34/34	0.87	0.17	2.59	9,11,58,64	0
3	TUD	B	302	34/34	0.90	0.16	2.43	10,12,109,116	0
3	TUD	D	302	34/34	0.82	0.16	2.05	17,20,57,65	0
3	TUD	C	302	34/34	0.85	0.17	1.86	11,15,80,89	0
2	NAP	D	301	48/48	0.92	0.17	1.44	18,25,107,111	0
2	NAP	C	301	48/48	0.94	0.15	1.31	16,21,61,64	0
2	NAP	A	301	48/48	0.93	0.16	1.27	17,23,76,79	0
4	GOL	B	303	6/6	0.93	0.10	-0.06	12,13,13,13	0
4	GOL	A	303	6/6	0.94	0.10	-0.58	14,15,15,16	0
4	GOL	C	303	6/6	0.96	0.08	-0.97	13,14,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.