



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:37 AM GMT

PDB ID : 3QWF
Title : Crystal structure of the 17beta-hydroxysteroiddehydrogenase from Cochliobolus lunatus
Authors : Cassetta, A.; Lamba, D.; Krastanova, I.; Stojan, J.; Lanisnik-Rizner, T.; Kristan, K.; Brunskole, M.
Deposited on : 2011-02-28
Resolution : 1.88 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

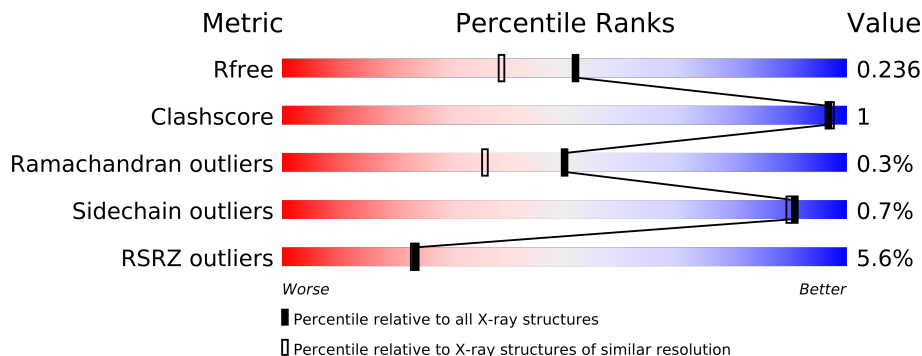
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.88 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}	66092	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	270	
1	B	270	
1	C	270	
1	D	270	
1	E	270	
1	F	270	
1	G	270	
1	H	270	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	302	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	G	301	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17526 atoms, of which 0 are hydrogen and 0 are deuterium.

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 17beta-hydroxysteroiddehydrogenase.

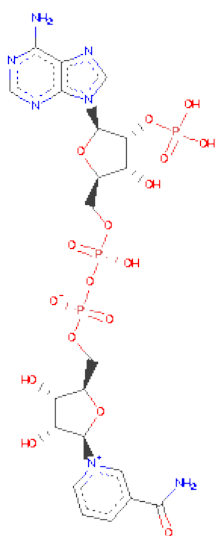
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	B	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	C	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	D	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	E	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	F	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	G	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	H	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	179	Total	O	0	0
			179	179		
4	C	191	Total	O	0	0
			191	191		
4	D	133	Total	O	0	0
			133	133		

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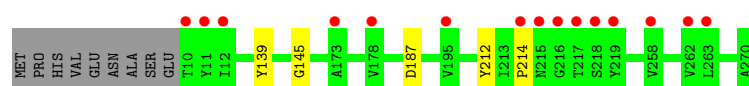
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	155	Total 155	O 155	0	0
4	F	157	Total 157	O 157	0	0
4	G	157	Total 157	O 157	0	0
4	H	149	Total 149	O 149	0	0

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 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.

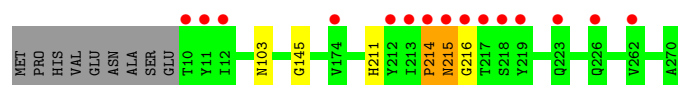
- Molecule 1: 17beta-hydroxysteroiddehydrogenase

Chain A: 



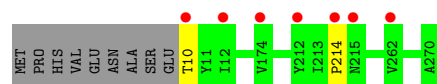
- Molecule 1: 17beta-hydroxysteroiddehydrogenase

Chain B: 



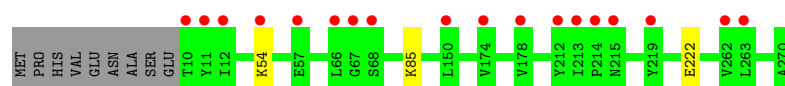
- Molecule 1: 17beta-hydroxysteroiddehydrogenase

Chain C: 



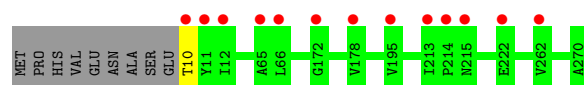
- Molecule 1: 17beta-hydroxysteroiddehydrogenase

Chain D: 



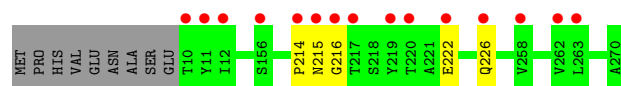
- Molecule 1: 17beta-hydroxysteroiddehydrogenase

Chain E: 

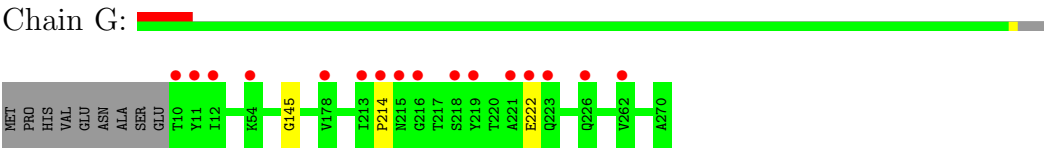


- Molecule 1: 17beta-hydroxysteroiddehydrogenase

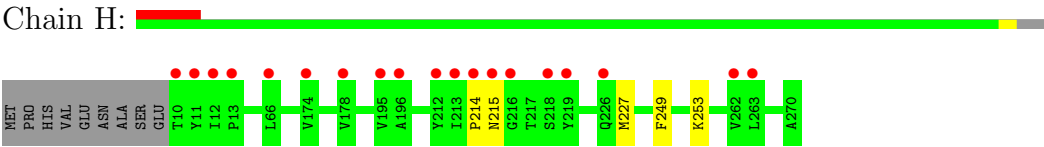
Chain F: 



● Molecule 1: 17beta-hydroxysteroiddehydrogenase



● Molecule 1: 17beta-hydroxysteroiddehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.52Å 67.83Å 138.89Å 84.20° 85.31° 66.57°	Depositor
Resolution (Å)	37.45 – 1.88 37.45 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.0 (37.45-1.88) 95.9 (37.45-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.194 0.213 , 0.236	Depositor DCC
R_{free} test set	8540 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 17.1	EDS
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 170172 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17526	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP

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	0.52	0/2010	0.55	0/2720
1	B	0.47	0/2010	0.54	0/2720
1	C	0.47	0/2010	0.54	0/2720
1	D	0.44	0/2010	0.52	0/2720
1	E	0.45	0/2010	0.53	0/2720
1	F	0.46	0/2010	0.55	0/2720
1	G	0.44	0/2010	0.53	0/2720
1	H	0.44	0/2010	0.51	0/2720
All	All	0.46	0/16080	0.53	0/21760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1971	0	0	3	0
1	B	1971	0	0	8	0
1	C	1971	0	0	0	0
1	D	1971	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1971	0	0	0	0
1	F	1971	0	0	0	0
1	G	1971	0	0	1	0
1	H	1971	0	0	2	0
2	A	12	0	16	2	0
2	B	12	0	16	1	0
2	C	6	0	8	0	0
2	D	6	0	8	1	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
2	G	6	0	8	1	0
2	H	6	0	8	1	0
3	A	48	0	25	0	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
3	E	48	0	25	0	0
3	F	48	0	25	0	0
3	G	48	0	25	0	0
3	H	48	0	25	0	0
4	A	193	0	0	2	0
4	B	179	0	0	1	0
4	C	191	0	0	0	0
4	D	133	0	0	0	0
4	E	155	0	0	0	0
4	F	157	0	0	0	0
4	G	157	0	0	0	0
4	H	149	0	0	1	0
All	All	17526	0	280	16	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (16) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:214:PRO:O	1:B:215:ASN:CG	2.04	0.96
2:A:302:GOL:H32	4:A:561:HOH:O	1.64	0.95
1:A:145:GLY:O	2:A:301:GOL:H32	1.88	0.73
1:B:211:HIS:NE2	4:B:575:HOH:O	2.24	0.71
1:B:215:ASN:OD1	1:B:216:GLY:N	2.25	0.70
1:B:214:PRO:O	1:B:215:ASN:ND2	2.29	0.66
1:B:145:GLY:O	2:B:302:GOL:H32	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:214:PRO:O	1:B:215:ASN:OD1	2.19	0.59
1:H:249:PHE:N	2:H:301:GOL:H32	2.22	0.55
1:D:222:GLU:CB	2:D:301:GOL:H11	2.42	0.50
1:B:214:PRO:C	1:B:215:ASN:CG	2.70	0.48
1:G:145:GLY:O	2:G:301:GOL:H32	2.13	0.48
1:H:253:LYS:NZ	4:H:522:HOH:O	2.46	0.47
1:A:139:TYR:OH	1:A:187:ASP:OD1	2.37	0.42
1:A:212:TYR:OH	4:A:461:HOH:O	2.21	0.42
1:B:215:ASN:CG	1:B:216:GLY:N	2.73	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	259/270 (96%)	250 (96%)	8 (3%)	1 (0%)	43	28
1	B	259/270 (96%)	250 (96%)	8 (3%)	1 (0%)	43	28
1	C	259/270 (96%)	248 (96%)	10 (4%)	1 (0%)	43	28
1	D	259/270 (96%)	251 (97%)	8 (3%)	0	100	100
1	E	259/270 (96%)	252 (97%)	7 (3%)	0	100	100
1	F	259/270 (96%)	251 (97%)	6 (2%)	2 (1%)	27	12
1	G	259/270 (96%)	250 (96%)	8 (3%)	1 (0%)	43	28
1	H	259/270 (96%)	249 (96%)	9 (4%)	1 (0%)	43	28
All	All	2072/2160 (96%)	2001 (97%)	64 (3%)	7 (0%)	50	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	214	PRO
1	A	214	PRO
1	G	214	PRO

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Mol	Chain	Res	Type
1	B	215	ASN
1	C	214	PRO
1	F	216	GLY
1	F	214	PRO

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	208/216 (96%)	208 (100%)	0	100	100
1	B	208/216 (96%)	206 (99%)	2 (1%)	85	83
1	C	208/216 (96%)	207 (100%)	1 (0%)	94	93
1	D	208/216 (96%)	206 (99%)	2 (1%)	85	83
1	E	208/216 (96%)	207 (100%)	1 (0%)	94	93
1	F	208/216 (96%)	205 (99%)	3 (1%)	78	73
1	G	208/216 (96%)	207 (100%)	1 (0%)	94	93
1	H	208/216 (96%)	206 (99%)	2 (1%)	85	83
All	All	1664/1728 (96%)	1652 (99%)	12 (1%)	91	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	103	ASN
1	B	214	PRO
1	C	10	THR
1	D	54	LYS
1	D	85	LYS
1	E	10	THR
1	F	215	ASN
1	F	222	GLU
1	F	226	GLN
1	G	222	GLU
1	H	215	ASN
1	H	227	MET

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 chains 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 ⓘ

18 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	GOL	A	301	-	5,5,5	0.30	0	5,5,5	0.56	0
2	GOL	A	302	-	5,5,5	0.37	0	5,5,5	0.31	0
3	NAP	A	303	-	52,52,52	1.45	6 (11%)	80,80,80	1.62	11 (13%)
2	GOL	B	301	-	5,5,5	0.36	0	5,5,5	0.48	0
2	GOL	B	302	-	5,5,5	0.32	0	5,5,5	0.49	0
3	NAP	B	303	-	52,52,52	1.42	8 (15%)	80,80,80	1.58	9 (11%)
2	GOL	C	301	-	5,5,5	0.35	0	5,5,5	0.26	0
3	NAP	C	302	-	52,52,52	1.44	6 (11%)	80,80,80	1.67	9 (11%)
2	GOL	D	301	-	5,5,5	0.42	0	5,5,5	0.57	0
3	NAP	D	302	-	52,52,52	1.42	6 (11%)	80,80,80	1.70	9 (11%)
2	GOL	E	301	-	5,5,5	0.30	0	5,5,5	0.33	0
3	NAP	E	302	-	52,52,52	1.38	4 (7%)	80,80,80	1.60	9 (11%)
2	GOL	F	301	-	5,5,5	0.28	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	F	302	-	52,52,52	1.30	4 (7%)	80,80,80	1.52	8 (10%)
2	GOL	G	301	-	5,5,5	0.30	0	5,5,5	0.48	0
3	NAP	G	302	-	52,52,52	1.46	6 (11%)	80,80,80	1.59	10 (12%)
2	GOL	H	301	-	5,5,5	0.41	0	5,5,5	0.27	0
3	NAP	H	302	-	52,52,52	1.37	6 (11%)	80,80,80	1.48	7 (8%)

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	GOL	A	301	-	-	0/4/4/4	0/0/0/0
2	GOL	A	302	-	-	0/4/4/4	0/0/0/0
3	NAP	A	303	-	-	0/35/67/67	0/3/5/5
2	GOL	B	301	-	-	0/4/4/4	0/0/0/0
2	GOL	B	302	-	-	0/4/4/4	0/0/0/0
3	NAP	B	303	-	-	0/35/67/67	0/3/5/5
2	GOL	C	301	-	-	0/4/4/4	0/0/0/0
3	NAP	C	302	-	-	0/35/67/67	0/3/5/5
2	GOL	D	301	-	-	0/4/4/4	0/0/0/0
3	NAP	D	302	-	-	0/35/67/67	0/3/5/5
2	GOL	E	301	-	-	0/4/4/4	0/0/0/0
3	NAP	E	302	-	-	0/35/67/67	0/3/5/5
2	GOL	F	301	-	-	0/4/4/4	0/0/0/0
3	NAP	F	302	-	-	0/35/67/67	0/3/5/5
2	GOL	G	301	-	-	0/4/4/4	0/0/0/0
3	NAP	G	302	-	-	0/35/67/67	0/3/5/5
2	GOL	H	301	-	-	0/4/4/4	0/0/0/0
3	NAP	H	302	-	-	0/35/67/67	0/3/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	NAP	C2N-N1N	5.54	1.42	1.35
3	C	302	NAP	C2N-N1N	5.48	1.42	1.35
3	A	303	NAP	C2N-N1N	5.19	1.42	1.35
3	H	302	NAP	C2N-N1N	5.17	1.41	1.35
3	G	302	NAP	O7N-C7N	5.16	1.36	1.24
3	D	302	NAP	O7N-C7N	5.09	1.36	1.24
3	F	302	NAP	O7N-C7N	4.87	1.35	1.24
3	A	303	NAP	O7N-C7N	4.87	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	NAP	O7N-C7N	4.78	1.35	1.24
3	H	302	NAP	O7N-C7N	4.70	1.35	1.24
3	B	303	NAP	C2N-N1N	4.62	1.41	1.35
3	G	302	NAP	C2N-N1N	4.60	1.41	1.35
3	E	302	NAP	O7N-C7N	4.58	1.34	1.24
3	F	302	NAP	C2N-N1N	4.54	1.41	1.35
3	D	302	NAP	C2N-N1N	4.50	1.41	1.35
3	C	302	NAP	O7N-C7N	4.16	1.33	1.24
3	F	302	NAP	C4A-N9A	-3.39	1.32	1.37
3	D	302	NAP	PA-O3	3.33	1.65	1.59
3	C	302	NAP	PA-O3	3.18	1.65	1.59
3	D	302	NAP	O4D-C1D	3.04	1.46	1.41
3	G	302	NAP	C4A-N9A	-2.95	1.33	1.37
3	C	302	NAP	C4A-N9A	-2.93	1.33	1.37
3	G	302	NAP	O4D-C1D	2.93	1.45	1.41
3	B	303	NAP	C4A-N9A	-2.92	1.33	1.37
3	H	302	NAP	C4A-N9A	-2.91	1.33	1.37
3	A	303	NAP	O4D-C1D	2.87	1.45	1.41
3	A	303	NAP	C4A-N9A	-2.86	1.33	1.37
3	E	302	NAP	O4D-C1D	2.83	1.45	1.41
3	G	302	NAP	O4B-C1B	2.73	1.45	1.41
3	D	302	NAP	C4A-N9A	-2.67	1.33	1.37
3	A	303	NAP	PA-O3	2.66	1.64	1.59
3	E	302	NAP	C4A-N9A	-2.61	1.33	1.37
3	H	302	NAP	O4D-C1D	2.55	1.45	1.41
3	B	303	NAP	O4B-C1B	2.43	1.45	1.41
3	B	303	NAP	PA-O3	2.39	1.64	1.59
3	B	303	NAP	PN-O5D	2.26	1.67	1.60
3	C	302	NAP	O4D-C1D	2.25	1.44	1.41
3	B	303	NAP	O4D-C1D	2.21	1.44	1.41
3	H	302	NAP	C6N-N1N	2.16	1.41	1.35
3	H	302	NAP	O4B-C1B	2.15	1.44	1.41
3	G	302	NAP	C6N-N1N	2.15	1.41	1.35
3	D	302	NAP	O4B-C1B	2.09	1.44	1.41
3	C	302	NAP	O4B-C1B	2.08	1.44	1.41
3	B	303	NAP	C3N-C7N	2.07	1.54	1.50
3	F	302	NAP	C6N-N1N	2.03	1.41	1.35
3	A	303	NAP	P2B-O2X	2.00	1.62	1.54

All (72) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	NAP	N3A-C2A-N1A	-8.79	121.36	128.71
3	G	302	NAP	N3A-C2A-N1A	-8.62	121.50	128.71
3	C	302	NAP	N3A-C2A-N1A	-8.58	121.53	128.71
3	F	302	NAP	N3A-C2A-N1A	-8.55	121.56	128.71
3	B	303	NAP	N3A-C2A-N1A	-8.36	121.72	128.71
3	E	302	NAP	N3A-C2A-N1A	-8.20	121.86	128.71
3	A	303	NAP	N3A-C2A-N1A	-8.08	121.96	128.71
3	H	302	NAP	N3A-C2A-N1A	-8.01	122.02	128.71
3	D	302	NAP	O4B-C1B-N9A	6.44	114.43	108.44
3	C	302	NAP	O4B-C1B-N9A	5.99	114.01	108.44
3	A	303	NAP	O4B-C1B-N9A	4.86	112.96	108.44
3	E	302	NAP	O4B-C1B-C2B	-4.45	102.79	106.95
3	E	302	NAP	N3A-C4A-N9A	4.42	133.42	125.43
3	E	302	NAP	O4B-C1B-N9A	4.39	112.53	108.44
3	B	303	NAP	N3A-C4A-N9A	4.36	133.30	125.43
3	D	302	NAP	N3A-C4A-N9A	4.33	133.26	125.43
3	G	302	NAP	O4B-C1B-N9A	4.16	112.31	108.44
3	B	303	NAP	O4B-C1B-C2B	-4.15	103.07	106.95
3	G	302	NAP	N3A-C4A-N9A	4.15	132.92	125.43
3	C	302	NAP	N3A-C4A-N9A	4.10	132.84	125.43
3	F	302	NAP	N3A-C4A-N9A	4.06	132.77	125.43
3	H	302	NAP	N3A-C4A-N9A	3.99	132.63	125.43
3	A	303	NAP	N3A-C4A-N9A	3.98	132.62	125.43
3	F	302	NAP	O4B-C1B-C2B	-3.72	103.47	106.95
3	H	302	NAP	O4B-C1B-N9A	3.64	111.83	108.44
3	A	303	NAP	C4A-C5A-N7A	-3.62	106.42	109.52
3	B	303	NAP	O4B-C1B-N9A	3.58	111.77	108.44
3	D	302	NAP	C5A-C4A-N3A	-2.98	119.20	125.70
3	D	302	NAP	C4A-C5A-N7A	-2.92	107.02	109.52
3	E	302	NAP	C5A-C4A-N3A	-2.91	119.37	125.70
3	B	303	NAP	C5A-C4A-N3A	-2.89	119.41	125.70
3	D	302	NAP	C4D-O4D-C1D	-2.89	106.61	109.75
3	G	302	NAP	O4B-C1B-C2B	-2.71	104.42	106.95
3	A	303	NAP	C5A-C4A-N3A	-2.67	119.89	125.70
3	C	302	NAP	C5A-C4A-N3A	-2.64	119.94	125.70
3	F	302	NAP	C4B-O4B-C1B	-2.64	106.89	109.75
3	H	302	NAP	C5A-C4A-N3A	-2.63	119.98	125.70
3	G	302	NAP	C5A-C4A-N3A	-2.58	120.08	125.70
3	C	302	NAP	C4B-O4B-C1B	-2.57	106.95	109.75
3	D	302	NAP	O4B-C1B-C2B	-2.56	104.55	106.95
3	E	302	NAP	C4A-C5A-N7A	-2.55	107.33	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	NAP	O4B-C1B-C2B	-2.55	104.56	106.95
3	G	302	NAP	O4D-C1D-N1N	2.55	110.56	107.95
3	D	302	NAP	C2A-N3A-C4A	2.50	121.14	114.01
3	F	302	NAP	C5A-C4A-N3A	-2.45	120.37	125.70
3	F	302	NAP	C4A-C5A-N7A	-2.45	107.43	109.52
3	G	302	NAP	C4B-O4B-C1B	-2.38	107.17	109.75
3	E	302	NAP	C6N-N1N-C2N	-2.37	119.36	122.04
3	H	302	NAP	C4A-C5A-N7A	-2.37	107.50	109.52
3	H	302	NAP	O4B-C1B-C2B	-2.36	104.74	106.95
3	A	303	NAP	O4B-C1B-C2B	-2.35	104.75	106.95
3	F	302	NAP	C8A-N9A-C4A	2.34	108.69	106.90
3	E	302	NAP	C2A-N3A-C4A	2.30	120.56	114.01
3	C	302	NAP	C2A-N3A-C4A	2.29	120.53	114.01
3	C	302	NAP	C2N-C3N-C4N	2.28	120.89	118.31
3	B	303	NAP	C2A-N3A-C4A	2.27	120.46	114.01
3	A	303	NAP	C4B-O4B-C1B	-2.24	107.31	109.75
3	A	303	NAP	C8A-N9A-C4A	2.24	108.61	106.90
3	C	302	NAP	C4A-C5A-N7A	-2.24	107.60	109.52
3	B	303	NAP	C4B-O4B-C1B	-2.23	107.32	109.75
3	B	303	NAP	C5B-C4B-C3B	-2.20	106.41	115.21
3	G	302	NAP	C4D-O4D-C1D	-2.19	107.37	109.75
3	A	303	NAP	C2A-N3A-C4A	2.18	120.22	114.01
3	D	302	NAP	C4B-O4B-C1B	-2.13	107.43	109.75
3	A	303	NAP	C6N-N1N-C2N	-2.12	119.65	122.04
3	E	302	NAP	C2N-C3N-C4N	2.11	120.70	118.31
3	G	302	NAP	C2A-N3A-C4A	2.11	120.00	114.01
3	B	303	NAP	C4A-C5A-N7A	-2.10	107.72	109.52
3	G	302	NAP	C4A-C5A-N7A	-2.09	107.73	109.52
3	A	303	NAP	N7A-C8A-N9A	-2.08	108.46	114.36
3	H	302	NAP	C2A-N3A-C4A	2.07	119.91	114.01
3	F	302	NAP	C2A-N3A-C4A	2.00	119.72	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	261/270 (96%)	0.36	15 (5%) 23 22	16, 28, 50, 60	0
1	B	261/270 (96%)	0.27	15 (5%) 23 22	17, 31, 65, 87	0
1	C	261/270 (96%)	0.18	7 (2%) 52 52	17, 30, 48, 65	0
1	D	261/270 (96%)	0.46	18 (6%) 17 16	20, 40, 69, 84	0
1	E	261/270 (96%)	0.29	13 (4%) 28 27	22, 33, 56, 72	0
1	F	261/270 (96%)	0.14	15 (5%) 23 22	22, 31, 55, 70	0
1	G	261/270 (96%)	0.27	16 (6%) 21 20	22, 34, 64, 86	0
1	H	261/270 (96%)	0.34	19 (7%) 15 14	22, 34, 58, 71	0
All	All	2088/2160 (96%)	0.29	118 (5%) 24 22	16, 33, 60, 87	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	213	ILE	7.9
1	B	215	ASN	7.7
1	G	214	PRO	6.9
1	D	10	THR	6.7
1	E	12	ILE	6.3
1	H	10	THR	6.0
1	H	12	ILE	5.2
1	A	214	PRO	5.2
1	A	215	ASN	5.0
1	F	10	THR	4.9
1	H	214	PRO	4.8
1	E	10	THR	4.8
1	G	12	ILE	4.7
1	B	10	THR	4.7
1	E	213	ILE	4.7
1	G	10	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	214	PRO	4.6
1	D	66	LEU	4.5
1	B	12	ILE	4.4
1	B	212	TYR	4.4
1	H	11	TYR	4.4
1	A	10	THR	4.4
1	H	213	ILE	4.2
1	F	219	TYR	4.1
1	B	11	TYR	4.0
1	E	11	TYR	4.0
1	F	11	TYR	3.9
1	C	10	THR	3.9
1	B	213	ILE	3.9
1	B	218	SER	3.9
1	B	217	THR	3.8
1	E	214	PRO	3.8
1	D	214	PRO	3.8
1	G	11	TYR	3.8
1	A	219	TYR	3.6
1	D	213	ILE	3.6
1	D	11	TYR	3.5
1	G	221	ALA	3.5
1	E	215	ASN	3.4
1	A	216	GLY	3.3
1	H	218	SER	3.3
1	A	12	ILE	3.2
1	G	226	GLN	3.2
1	F	215	ASN	3.2
1	D	12	ILE	3.2
1	D	215	ASN	3.1
1	E	66	LEU	3.1
1	E	222	GLU	3.1
1	F	217	THR	3.1
1	E	262	VAL	3.0
1	H	263	LEU	3.0
1	G	222	GLU	3.0
1	A	11	TYR	3.0
1	C	262	VAL	2.9
1	H	226	GLN	2.9
1	C	212	TYR	2.8
1	F	226	GLN	2.8
1	F	214	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	219	TYR	2.8
1	H	215	ASN	2.8
1	D	212	TYR	2.7
1	D	68	SER	2.7
1	F	220	THR	2.7
1	D	67	GLY	2.7
1	B	219	TYR	2.7
1	A	262	VAL	2.7
1	H	174	VAL	2.6
1	H	216	GLY	2.6
1	E	178	VAL	2.6
1	G	262	VAL	2.6
1	C	12	ILE	2.6
1	B	226	GLN	2.6
1	H	262	VAL	2.6
1	C	215	ASN	2.6
1	G	215	ASN	2.6
1	F	216	GLY	2.5
1	D	57	GLU	2.5
1	D	219	TYR	2.5
1	G	218	SER	2.5
1	D	262	VAL	2.5
1	F	263	LEU	2.5
1	G	216	GLY	2.5
1	A	258	VAL	2.4
1	F	262	VAL	2.4
1	H	212	TYR	2.4
1	H	66	LEU	2.4
1	A	263	LEU	2.4
1	F	12	ILE	2.4
1	C	214	PRO	2.3
1	B	262	VAL	2.3
1	B	216	GLY	2.3
1	A	178	VAL	2.3
1	B	174	VAL	2.3
1	F	258	VAL	2.2
1	A	217	THR	2.2
1	A	218	SER	2.2
1	E	172	GLY	2.2
1	H	219	TYR	2.2
1	D	178	VAL	2.2
1	F	156	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	196	ALA	2.2
1	H	195	VAL	2.2
1	D	263	LEU	2.1
1	G	54	LYS	2.1
1	E	65	ALA	2.1
1	D	150	LEU	2.1
1	A	173	ALA	2.1
1	G	178	VAL	2.1
1	B	223	GLN	2.1
1	E	195	VAL	2.1
1	H	13	PRO	2.1
1	A	195	VAL	2.1
1	G	223	GLN	2.0
1	D	54	LYS	2.0
1	F	222	GLU	2.0
1	C	174	VAL	2.0
1	D	174	VAL	2.0
1	H	178	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	302	6/6	0.23	3.71	46,49,50,51	0
2	GOL	G	301	6/6	0.19	3.01	49,51,51,52	0
2	GOL	D	301	6/6	0.19	1.94	30,36,37,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	F	301	6/6	0.17	1.90	37,39,40,42	0
3	NAP	G	302	48/48	0.15	1.46	10,12,13,14	0
2	GOL	B	302	6/6	0.14	0.95	31,32,33,34	0
2	GOL	E	301	6/6	0.12	0.74	44,49,50,51	0
2	GOL	B	301	6/6	0.13	0.68	37,41,42,44	0
2	GOL	H	301	6/6	0.15	0.48	43,47,48,49	0
3	NAP	D	302	48/48	0.12	0.31	9,11,12,13	0
3	NAP	H	302	48/48	0.12	0.27	9,11,12,14	0
2	GOL	A	301	6/6	0.11	0.18	42,45,47,48	0
3	NAP	E	302	48/48	0.11	0.12	10,12,14,14	0
2	GOL	C	301	6/6	0.11	-0.21	32,37,37,38	0
3	NAP	C	302	48/48	0.09	-0.53	19,25,29,30	0
3	NAP	F	302	48/48	0.09	-0.54	7,11,12,13	0
3	NAP	B	303	48/48	0.08	-0.64	23,29,35,35	0
3	NAP	A	303	48/48	0.06	-1.54	8,10,12,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.