



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:10 PM GMT

PDB ID : 1XSE
Title : Crystal Structure of Guinea Pig 11beta-HydroxysteroidDehydrogenase Type 1
Authors : Ogg, D.; Elleby, B.; Norstrom, C.; Stefansson, K.; Abrahmsen, L.; Oppermann, U.; Svensson, S.
Deposited on : 2004-10-19
Resolution : 2.50 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>

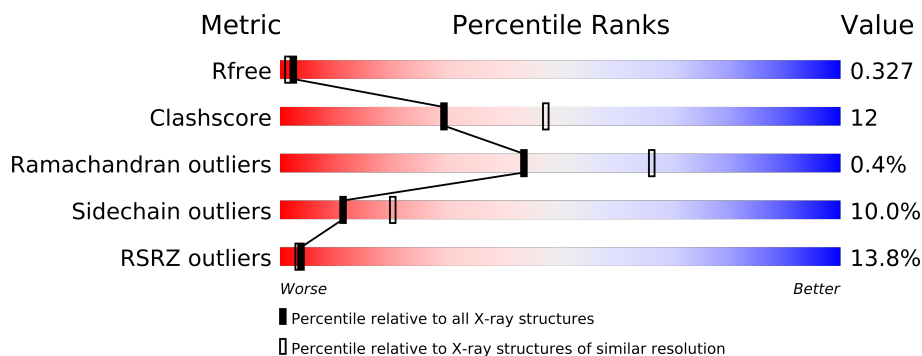
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	295	
1	B	295	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4655 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 11beta-hydroxysteroiddehydrogenase type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2105	1351	351	388	15			
1	B	274	Total	C	N	O	S	0	0	0
			2105	1351	351	388	15			

There are 42 discrepancies between the modelled and reference sequences:

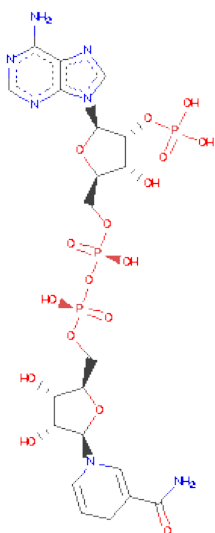
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	CLONING ARTIFACT	UNP Q6QLL4
A	4	GLY	-	CLONING ARTIFACT	UNP Q6QLL4
A	5	SER	-	CLONING ARTIFACT	UNP Q6QLL4
A	6	SER	-	CLONING ARTIFACT	UNP Q6QLL4
A	7	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
A	8	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
A	9	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
A	10	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
A	11	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
A	12	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
A	13	SER	-	CLONING ARTIFACT	UNP Q6QLL4
A	14	SER	-	CLONING ARTIFACT	UNP Q6QLL4
A	15	GLY	-	CLONING ARTIFACT	UNP Q6QLL4
A	16	LEU	-	CLONING ARTIFACT	UNP Q6QLL4
A	17	VAL	-	CLONING ARTIFACT	UNP Q6QLL4
A	18	PRO	-	CLONING ARTIFACT	UNP Q6QLL4
A	19	ARG	-	CLONING ARTIFACT	UNP Q6QLL4
A	20	GLY	-	CLONING ARTIFACT	UNP Q6QLL4
A	21	SER	-	CLONING ARTIFACT	UNP Q6QLL4
A	22	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
A	23	MET	-	CLONING ARTIFACT	UNP Q6QLL4
B	3	MET	-	CLONING ARTIFACT	UNP Q6QLL4
B	4	GLY	-	CLONING ARTIFACT	UNP Q6QLL4
B	5	SER	-	CLONING ARTIFACT	UNP Q6QLL4
B	6	SER	-	CLONING ARTIFACT	UNP Q6QLL4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
B	8	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
B	9	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
B	10	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
B	11	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
B	12	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
B	13	SER	-	CLONING ARTIFACT	UNP Q6QLL4
B	14	SER	-	CLONING ARTIFACT	UNP Q6QLL4
B	15	GLY	-	CLONING ARTIFACT	UNP Q6QLL4
B	16	LEU	-	CLONING ARTIFACT	UNP Q6QLL4
B	17	VAL	-	CLONING ARTIFACT	UNP Q6QLL4
B	18	PRO	-	CLONING ARTIFACT	UNP Q6QLL4
B	19	ARG	-	CLONING ARTIFACT	UNP Q6QLL4
B	20	GLY	-	CLONING ARTIFACT	UNP Q6QLL4
B	21	SER	-	CLONING ARTIFACT	UNP Q6QLL4
B	22	HIS	-	CLONING ARTIFACT	UNP Q6QLL4
B	23	MET	-	CLONING ARTIFACT	UNP Q6QLL4

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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		

- Molecule 3 is water.

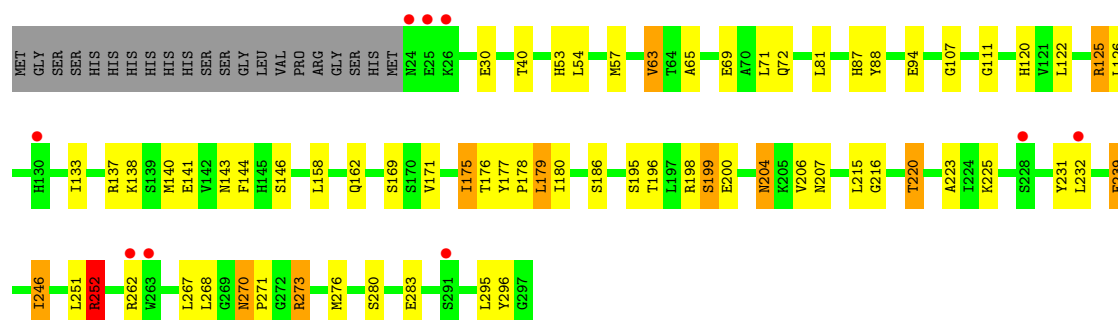
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	235	Total 235	O 235	0	0
3	B	114	Total 114	O 114	0	0

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.

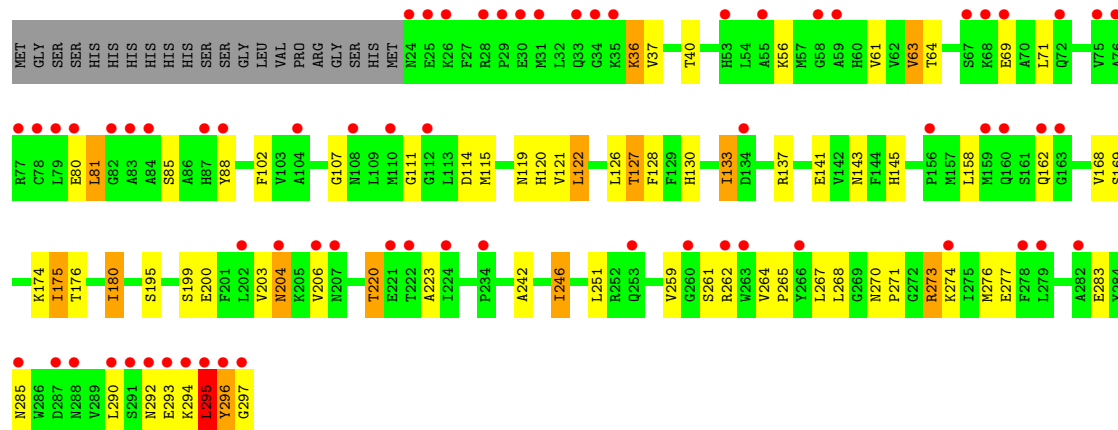
- Molecule 1: 11beta-hydroxysteroiddehydrogenase type 1

Chain A:



- Molecule 1: 11beta-hydroxysteroiddehydrogenase type 1

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.39Å 118.39Å 184.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 9.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (10.00-2.50) 99.7 (9.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0001	Depositor
R, R_{free}	0.192 , 0.267 0.255 , 0.327	Depositor DCC
R_{free} test set	1162 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 78.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 22609 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4655	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: NDP

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	0.75	0/2145	0.84	5/2897 (0.2%)
1	B	0.64	1/2145 (0.0%)	0.77	3/2897 (0.1%)
All	All	0.70	1/4290 (0.0%)	0.81	8/5794 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLU	CG-CD	6.45	1.61	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	252	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	204	ASN	N-CA-C	7.05	130.04	111.00
1	B	204	ASN	N-CA-C	6.35	128.14	111.00
1	A	198	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	252	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	180	ILE	N-CA-C	5.67	126.30	111.00
1	A	198	ARG	NE-CZ-NH1	5.37	122.98	120.30

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	2105	0	2135	63	0
1	B	2105	0	2135	56	0
2	A	48	0	26	4	0
2	B	48	0	26	3	0
3	A	235	0	0	5	0
3	B	114	0	0	6	0
All	All	4655	0	4322	106	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 12.

All (106) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:VAL:HB	3:A:1518:HOH:O	1.25	1.30
1:B:122:LEU:H	1:B:143:ASN:HD21	1.06	1.00
1:A:140:MET:HE1	1:A:144:PHE:CD2	2.12	0.84
1:A:122:LEU:H	1:A:143:ASN:HD21	1.28	0.80
1:B:220:THR:HG22	1:B:223:ALA:H	1.49	0.77
1:A:276:MET:CE	1:B:267:LEU:HD12	2.15	0.76
1:B:122:LEU:H	1:B:143:ASN:ND2	1.84	0.75
1:A:125:ARG:CG	1:A:125:ARG:HH11	2.01	0.74
1:A:220:THR:HG22	1:A:223:ALA:H	1.53	0.72
1:A:140:MET:HE3	1:A:144:PHE:HB3	1.74	0.70
1:A:162:GLN:O	1:A:252:ARG:NH2	2.25	0.69
1:A:162:GLN:HG2	1:A:207:ASN:HB3	1.74	0.69
1:A:125:ARG:HH11	1:A:125:ARG:HG3	1.56	0.69
1:A:140:MET:CE	1:A:144:PHE:CD2	2.75	0.69
1:B:220:THR:HG21	2:B:2300:NDP:O2N	1.93	0.68
1:A:207:ASN:HA	3:A:1342:HOH:O	1.94	0.68
1:A:63:VAL:HG13	1:A:71:LEU:HD22	1.75	0.68
1:A:87:HIS:HD2	3:A:1306:HOH:O	1.76	0.68
1:A:206:VAL:O	1:A:207:ASN:HB2	1.94	0.67
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.79	0.64
1:A:273:ARG:HD3	1:B:175:ILE:HG13	1.80	0.63
1:A:125:ARG:CB	1:A:125:ARG:HH11	2.11	0.62
1:A:120:HIS:HE1	1:A:146:SER:OG	1.83	0.62
1:A:175:ILE:HD13	1:A:268:LEU:CD2	2.30	0.61
1:A:276:MET:HE1	1:B:267:LEU:HD12	1.83	0.60
1:B:119:ASN:HD22	1:B:168:VAL:HG21	1.67	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:40:THR:O	1:B:119:ASN:HB3	2.01	0.59
1:A:270:ASN:HB3	1:B:270:ASN:CB	2.33	0.58
1:A:267:LEU:HD12	1:B:276:MET:CE	2.34	0.57
1:B:292:ASN:O	1:B:295:LEU:HD12	2.04	0.57
1:A:239:GLU:HB3	3:A:1313:HOH:O	2.03	0.57
1:A:137:ARG:HH22	1:B:141:GLU:CD	2.08	0.57
1:A:232:LEU:HD11	1:B:285:ASN:HB2	1.86	0.57
1:B:40:THR:HB	1:B:120:HIS:HD2	1.70	0.57
1:A:169:SER:O	2:A:1300:NDP:H6N	2.05	0.56
1:B:295:LEU:HD13	1:B:296:TYR:N	2.21	0.56
1:A:200:GLU:O	1:A:204:ASN:HB2	2.07	0.55
1:B:174:LYS:O	1:B:175:ILE:HD12	2.07	0.54
1:A:175:ILE:CD1	1:A:268:LEU:HD23	2.39	0.53
1:A:125:ARG:HG3	1:A:125:ARG:NH1	2.24	0.52
1:A:122:LEU:H	1:A:143:ASN:ND2	2.04	0.52
1:A:216:GLY:O	2:A:1300:NDP:H42N	2.10	0.52
1:B:40:THR:CB	1:B:120:HIS:HD2	2.23	0.52
1:A:178:PRO:O	1:A:179:LEU:HB2	2.10	0.52
1:B:296:TYR:HD2	1:B:297:GLY:N	2.08	0.52
1:A:175:ILE:CD1	1:A:268:LEU:CD2	2.88	0.51
1:A:220:THR:HG21	2:A:1300:NDP:O2N	2.11	0.51
1:B:63:VAL:HG12	1:B:71:LEU:HD22	1.93	0.51
1:A:206:VAL:O	1:A:207:ASN:CB	2.55	0.50
1:A:231:TYR:CE1	1:B:283:GLU:HB3	2.46	0.50
1:B:295:LEU:HD13	1:B:296:TYR:H	1.75	0.50
1:A:126:LEU:CD2	1:A:180:ILE:CG2	2.90	0.50
1:A:53:HIS:O	1:A:57:MET:HE3	2.12	0.49
1:B:85:SER:HB3	3:B:2414:HOH:O	2.12	0.49
1:A:162:GLN:HG2	1:A:207:ASN:CB	2.41	0.49
1:B:273:ARG:HG2	3:B:2334:HOH:O	2.12	0.49
1:B:40:THR:HG1	1:B:119:ASN:H	1.60	0.49
1:B:63:VAL:O	1:B:88:TYR:HA	2.13	0.49
1:B:64:THR:HB	1:B:102:PHE:CE1	2.48	0.48
1:B:36:LYS:HG2	1:B:114:ASP:OD2	2.13	0.48
1:B:37:VAL:HG22	1:B:115:MET:HB3	1.95	0.48
1:A:175:ILE:HD13	1:A:268:LEU:HD23	1.94	0.48
1:B:273:ARG:HD2	1:B:277:GLU:OE2	2.13	0.48
1:B:40:THR:HA	1:B:64:THR:HG22	1.96	0.47
1:B:169:SER:O	2:B:2300:NDP:H6N	2.14	0.47
1:A:54:LEU:HA	1:A:57:MET:HE3	1.95	0.47
1:B:290:LEU:HA	3:B:2340:HOH:O	2.14	0.47
1:B:107:GLY:O	1:B:111:GLY:N	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:VAL:O	1:A:88:TYR:HA	2.14	0.47
1:B:296:TYR:CD2	1:B:297:GLY:N	2.83	0.47
1:A:195:SER:HB2	1:B:176:THR:HG21	1.96	0.46
1:A:141:GLU:OE2	1:B:137:ARG:NH2	2.49	0.46
1:A:246:ILE:HD12	1:A:246:ILE:HG21	1.56	0.46
1:A:94:GLU:OE2	1:A:138:LYS:HE3	2.16	0.46
1:A:126:LEU:HD22	1:A:180:ILE:CG2	2.47	0.45
1:A:280:SER:O	1:A:283:GLU:HB2	2.16	0.45
1:A:107:GLY:O	1:A:111:GLY:N	2.49	0.45
1:B:121:VAL:HB	2:B:2300:NDP:H3D	1.97	0.45
1:A:270:ASN:HB3	1:B:270:ASN:HB2	1.98	0.45
1:B:63:VAL:CG1	1:B:71:LEU:HD22	2.47	0.45
1:B:270:ASN:HA	1:B:271:PRO:HD2	1.60	0.44
1:B:293:GLU:HG2	3:B:2340:HOH:O	2.18	0.44
1:B:264:VAL:N	1:B:265:PRO:HD2	2.33	0.44
1:B:242:ALA:O	1:B:246:ILE:HG12	2.18	0.44
1:B:133:ILE:HD11	3:B:2316:HOH:O	2.17	0.44
1:B:206:VAL:HA	3:B:2406:HOH:O	2.17	0.43
1:B:174:LYS:C	1:B:175:ILE:HD12	2.39	0.43
1:A:30:GLU:CD	1:A:30:GLU:H	2.21	0.43
1:B:127:THR:HG23	1:B:128:PHE:O	2.19	0.43
1:A:143:ASN:HB2	1:A:186:SER:HB2	2.01	0.42
3:A:1500:HOH:O	1:B:145:HIS:CD2	2.73	0.42
1:B:56:LYS:HG3	1:B:81:LEU:HG	2.02	0.42
1:A:143:ASN:N	1:A:143:ASN:HD22	2.17	0.42
1:B:200:GLU:O	1:B:204:ASN:HB2	2.19	0.42
1:A:215:LEU:HB2	2:A:1300:NDP:C5N	2.49	0.41
1:A:196:THR:O	1:A:199:SER:HB2	2.20	0.41
1:A:246:ILE:HD13	1:A:246:ILE:HG23	1.66	0.41
1:A:63:VAL:HG13	1:A:71:LEU:CD2	2.47	0.41
1:B:175:ILE:HD13	1:B:268:LEU:CD2	2.51	0.41
1:A:270:ASN:HA	1:A:271:PRO:HD2	1.77	0.41
1:A:175:ILE:HG22	1:A:177:TYR:CE1	2.56	0.41
1:A:126:LEU:HD22	1:A:180:ILE:HG23	2.03	0.41
1:A:175:ILE:HG13	1:B:273:ARG:HB2	2.03	0.41
1:B:128:PHE:O	1:B:130:HIS:CD2	2.73	0.40
1:A:176:THR:HG21	1:B:195:SER:HB2	2.03	0.40
1:B:180:ILE:O	1:B:180:ILE:HG13	2.21	0.40

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	272/295 (92%)	260 (96%)	10 (4%)	2 (1%)	30	50
1	B	272/295 (92%)	263 (97%)	9 (3%)	0	100	100
All	All	544/590 (92%)	523 (96%)	19 (4%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ALA
1	A	270	ASN

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	224/242 (93%)	204 (91%)	20 (9%)	14	26
1	B	224/242 (93%)	199 (89%)	25 (11%)	9	15
All	All	448/484 (93%)	403 (90%)	45 (10%)	11	20

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	69	GLU
1	A	72	GLN
1	A	81	LEU
1	A	125	ARG
1	A	133	ILE
1	A	158	LEU

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Mol	Chain	Res	Type
1	A	175	ILE
1	A	179	LEU
1	A	199	SER
1	A	220	THR
1	A	225	LYS
1	A	239	GLU
1	A	246	ILE
1	A	251	LEU
1	A	252	ARG
1	A	262	ARG
1	A	273	ARG
1	A	295	LEU
1	A	296	TYR
1	B	36	LYS
1	B	61	VAL
1	B	63	VAL
1	B	69	GLU
1	B	81	LEU
1	B	122	LEU
1	B	126	LEU
1	B	127	THR
1	B	133	ILE
1	B	158	LEU
1	B	162	GLN
1	B	175	ILE
1	B	199	SER
1	B	203	VAL
1	B	220	THR
1	B	246	ILE
1	B	251	LEU
1	B	259	VAL
1	B	261	SER
1	B	262	ARG
1	B	273	ARG
1	B	274	LYS
1	B	294	LYS
1	B	295	LEU
1	B	296	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	143	ASN
1	B	72	GLN
1	B	119	ASN
1	B	120	HIS
1	B	130	HIS
1	B	143	ASN
1	B	270	ASN

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 ⓘ

2 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	NDP	A	1300	-	52,52,52	1.89	7 (13%)	80,80,80	1.75	13 (16%)
2	NDP	B	2300	-	52,52,52	1.85	8 (15%)	80,80,80	1.75	14 (17%)

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	NDP	A	1300	-	-	0/35/77/77	0/3/5/5
2	NDP	B	2300	-	-	0/35/77/77	0/3/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	NDP	O7N-C7N	8.34	1.46	1.24
2	B	2300	NDP	O7N-C7N	7.89	1.45	1.24
2	A	1300	NDP	C4N-C3N	-5.34	1.39	1.50
2	B	2300	NDP	C4N-C3N	-5.27	1.40	1.50
2	A	1300	NDP	C4N-C5N	-4.83	1.38	1.49
2	B	2300	NDP	C7N-N7N	4.44	1.47	1.33
2	B	2300	NDP	C4N-C5N	-4.18	1.39	1.49
2	A	1300	NDP	C5A-C4A	3.40	1.48	1.40
2	A	1300	NDP	C7N-N7N	3.38	1.44	1.33
2	B	2300	NDP	C6N-C5N	3.33	1.40	1.33
2	A	1300	NDP	C6N-C5N	2.95	1.39	1.33
2	A	1300	NDP	C2N-C3N	2.83	1.40	1.34
2	B	2300	NDP	C5A-C4A	2.74	1.46	1.40
2	B	2300	NDP	C2N-C3N	2.71	1.40	1.34
2	B	2300	NDP	C4A-N9A	-2.40	1.34	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NDP	N3A-C2A-N1A	-9.44	120.82	128.71
2	B	2300	NDP	N3A-C2A-N1A	-6.95	122.90	128.71
2	B	2300	NDP	O4B-C1B-N9A	6.13	114.14	108.44
2	B	2300	NDP	N3A-C4A-N9A	5.01	134.48	125.43
2	A	1300	NDP	N3A-C4A-N9A	4.67	133.86	125.43
2	B	2300	NDP	C4A-C5A-N7A	-3.71	106.35	109.52
2	B	2300	NDP	O4D-C1D-N1N	3.65	115.77	108.05
2	B	2300	NDP	O4B-C1B-C2B	-3.21	103.95	106.95
2	A	1300	NDP	C4A-C5A-N7A	-3.05	106.91	109.52
2	B	2300	NDP	C5A-C4A-N3A	-3.01	119.14	125.70
2	B	2300	NDP	PN-O3-PA	-2.88	123.25	131.68
2	B	2300	NDP	C3N-C2N-N1N	-2.87	118.98	123.05
2	A	1300	NDP	O4B-C1B-N9A	2.85	111.09	108.44
2	A	1300	NDP	C2A-N1A-C6A	2.72	123.68	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2300	NDP	C4N-C5N-C6N	-2.68	117.69	122.61
2	A	1300	NDP	C3N-C2N-N1N	-2.65	119.29	123.05
2	A	1300	NDP	C8A-N9A-C4A	2.59	108.87	106.90
2	A	1300	NDP	PN-O3-PA	-2.52	124.30	131.68
2	B	2300	NDP	C5N-C4N-C3N	2.45	119.25	112.60
2	A	1300	NDP	C5A-C4A-N3A	-2.44	120.39	125.70
2	B	2300	NDP	O3X-P2B-O2X	2.41	117.00	107.61
2	A	1300	NDP	O4D-C1D-N1N	2.38	113.09	108.05
2	A	1300	NDP	O2B-C2B-C1B	2.36	119.08	110.36
2	B	2300	NDP	C8A-N9A-C4A	2.25	108.62	106.90
2	A	1300	NDP	C4N-C5N-C6N	-2.09	118.78	122.61
2	A	1300	NDP	C5N-C4N-C3N	2.07	118.22	112.60
2	B	2300	NDP	C2A-N3A-C4A	2.06	119.89	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	274/295 (92%)	0.50	9 (3%) 44 45	48, 55, 63, 79	0
1	B	274/295 (92%)	1.15	67 (24%) 1 1	49, 56, 64, 78	0
All	All	548/590 (92%)	0.83	76 (13%) 4 3	48, 56, 63, 79	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	GLY	10.9
1	B	294	LYS	7.6
1	B	24	ASN	7.3
1	B	295	LEU	6.4
1	B	104	ALA	6.3
1	B	296	TYR	6.0
1	B	290	LEU	5.8
1	B	108	ASN	5.3
1	A	263	TRP	5.1
1	B	202	LEU	4.8
1	B	156	PRO	4.7
1	B	160	GLN	4.5
1	A	24	ASN	4.4
1	B	82	GLY	4.4
1	B	266	TYR	4.2
1	B	293	GLU	4.2
1	B	28	ARG	4.1
1	B	288	ASN	4.1
1	B	278	PHE	4.0
1	B	80	GLU	4.0
1	B	207	ASN	3.9
1	B	67	SER	3.9
1	B	263	TRP	3.7
1	B	287	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	130	HIS	3.6
1	B	79	LEU	3.5
1	B	69	GLU	3.5
1	B	76	ALA	3.3
1	B	292	ASN	3.2
1	B	25	GLU	3.2
1	B	159	MET	3.1
1	B	162	GLN	3.1
1	B	72	GLN	3.0
1	B	224	ILE	3.0
1	A	228	SER	2.9
1	B	204	ASN	2.8
1	B	58	GLY	2.8
1	B	253	GLN	2.8
1	A	262	ARG	2.8
1	B	26	LYS	2.8
1	B	31	MET	2.8
1	B	30	GLU	2.8
1	B	83	ALA	2.8
1	B	291	SER	2.7
1	B	78	CYS	2.7
1	B	262	ARG	2.7
1	A	232	LEU	2.7
1	B	75	VAL	2.6
1	B	134	ASP	2.6
1	B	87	HIS	2.6
1	B	88	TYR	2.6
1	A	291	SER	2.5
1	B	112	GLY	2.5
1	B	33	GLN	2.5
1	B	206	VAL	2.5
1	A	26	LYS	2.4
1	A	25	GLU	2.4
1	B	110	MET	2.4
1	B	55	ALA	2.3
1	B	59	ALA	2.3
1	B	274	LYS	2.3
1	B	221	GLU	2.3
1	B	29	PRO	2.2
1	B	282	ALA	2.2
1	B	35	LYS	2.2
1	B	68	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	34	GLY	2.1
1	B	285	ASN	2.1
1	B	53	HIS	2.1
1	B	222	THR	2.1
1	B	234	PRO	2.1
1	B	77	ARG	2.1
1	B	84	ALA	2.0
1	B	279	LEU	2.0
1	B	163	GLY	2.0
1	B	260	GLY	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	NDP	A	1300	48/48	0.17	0.08	50,54,59,61	0
2	NDP	B	2300	48/48	0.13	-0.84	52,55,61,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.