



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:09 PM GMT

PDB ID : 3D90
Title : Crystal structure of the human progesterone receptor ligand-binding domain bound to levonorgestrel
Authors : Petit-Topin, I.; Turque, N.; Ulman, A.; Gainer, E.; Rafestin-Oblin, M.E.; Fagart, J.
Deposited on : 2008-05-26
Resolution : 2.26 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>

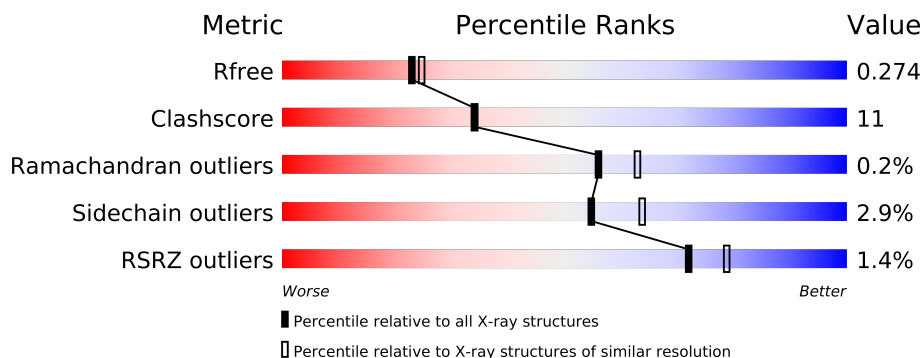
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.26 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	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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	258	
1	B	258	

2 Entry composition i

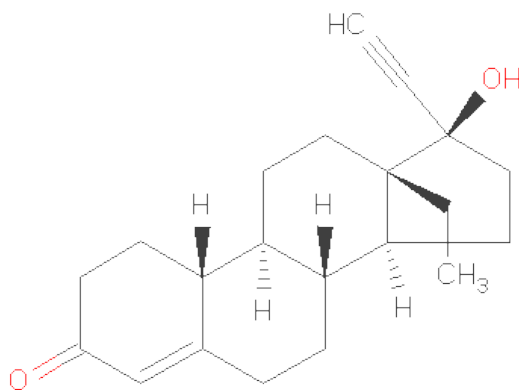
There are 3 unique types of molecules in this entry. The entry contains 4365 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Progesterone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1981	1286	326	355	14			
1	B	249	Total	C	N	O	S	0	0	0
			1986	1287	329	356	14			

- Molecule 2 is 13-BETA-ETHYL-17-ALPHA-ETHYNYL-17-BETA-HYDROXYGON-4-EN-3-ONE (three-letter code: NOG) (formula: $C_{21}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	21	2		
2	B	1	Total	C	O	0	0
			23	21	2		

- Molecule 3 is water.

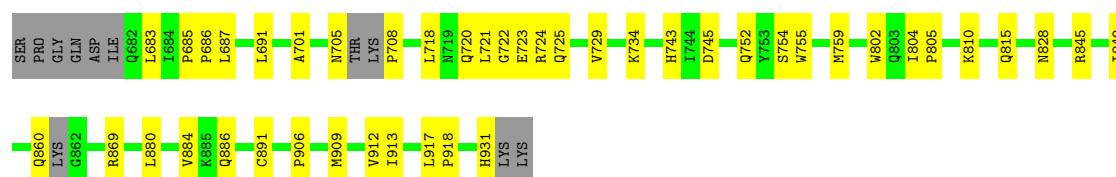
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	208	Total 208	O 208	0	0
3	B	144	Total 144	O 144	0	0

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.

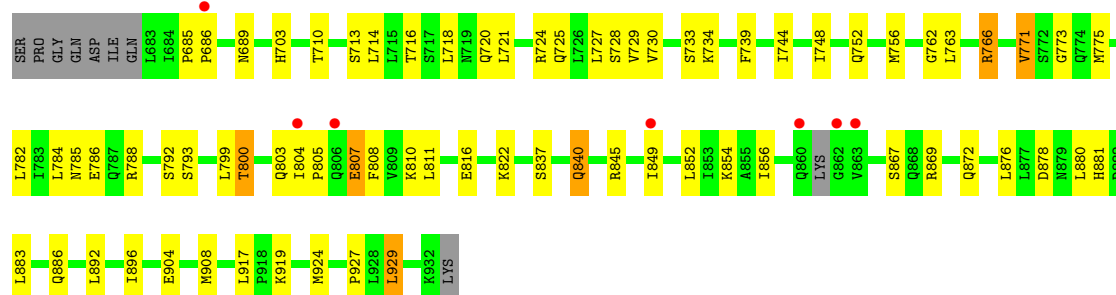
• Molecule 1: Progesterone receptor

Chain A: 



• Molecule 1: Progesterone receptor

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.87Å 65.31Å 70.62Å 90.00° 96.01° 90.00°	Depositor
Resolution (Å)	47.83 – 2.26 47.83 – 2.26	Depositor EDS
% Data completeness (in resolution range)	80.9 (47.83-2.26) 80.9 (47.83-2.26)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.27Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.279 0.233 , 0.274	Depositor DCC
R_{free} test set	1058 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.934	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 20345 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4365	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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: NOG

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	0.35	0/2022	0.59	1/2734 (0.0%)
1	B	0.32	0/2028	0.54	0/2746
All	All	0.33	0/4050	0.57	1/5480 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	PRO	CA-N-CD	-6.01	103.09	111.50

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	1981	0	2018	32	0
1	B	1986	0	2007	56	0
2	A	23	0	26	4	0
2	B	23	0	26	1	0
3	A	208	0	0	8	0
3	B	144	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4365	0	4077	88	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 11.

All (88) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:762:GLY:O	1:B:766:ARG:NH2	1.86	1.09
1:B:766:ARG:HG3	1:B:766:ARG:HH21	1.12	1.06
1:B:766:ARG:HH21	1:B:766:ARG:CG	1.69	1.04
1:B:762:GLY:C	1:B:766:ARG:HH22	1.66	0.98
1:A:828:ASN:OD1	1:A:845:ARG:NH1	2.00	0.94
1:B:766:ARG:NH2	1:B:766:ARG:HG3	1.87	0.82
1:B:784:LEU:HA	1:B:788:ARG:HD3	1.59	0.81
1:A:754:SER:HB3	3:A:3019:HOH:O	1.84	0.76
1:B:766:ARG:NH1	3:B:3084:HOH:O	2.22	0.72
1:B:800:THR:HG22	1:B:883:LEU:HG	1.73	0.70
1:B:766:ARG:CB	1:B:766:ARG:HH21	2.04	0.69
1:B:716:THR:HG23	1:B:904:GLU:HB3	1.76	0.67
1:B:766:ARG:NH2	1:B:766:ARG:HB2	2.10	0.67
1:B:766:ARG:NH2	1:B:766:ARG:CG	2.42	0.65
1:A:701:ALA:HB2	1:A:721:LEU:HD13	1.77	0.65
1:B:792:SER:O	1:B:793:SER:HB3	1.96	0.64
1:B:725:GLN:O	1:B:729:VAL:HG23	1.98	0.64
1:A:752:GLN:HG2	1:A:912:VAL:HG12	1.79	0.63
1:A:918:PRO:HD2	3:A:3070:HOH:O	2.01	0.60
1:B:799:LEU:O	1:B:803:GLN:HG3	2.02	0.59
1:A:721:LEU:HD23	2:A:1001:NOG:HC21	1.84	0.59
1:B:892:LEU:O	1:B:896:ILE:HG12	2.04	0.57
1:B:800:THR:HA	1:B:803:GLN:OE1	2.05	0.57
1:B:766:ARG:NH2	1:B:766:ARG:CB	2.66	0.57
1:B:837:SER:HB3	1:B:840:GLN:HG3	1.88	0.56
1:B:748:ILE:O	1:B:752:GLN:HG3	2.06	0.56
1:B:721:LEU:O	1:B:725:GLN:HG3	2.07	0.55
1:A:755:TRP:CE3	1:A:909:MET:HE1	2.41	0.55
1:B:710:THR:H	1:B:713:SER:HB3	1.71	0.55
1:B:685:PRO:HG2	1:B:854:LYS:HB3	1.88	0.55
1:B:869:ARG:HA	1:B:872:GLN:HG2	1.89	0.54
1:B:703:HIS:ND1	1:B:782:LEU:HD13	2.23	0.53
1:A:687:LEU:O	1:A:691:LEU:HG	2.09	0.52
1:B:718:LEU:HB3	2:B:2001:NOG:H112	1.91	0.51
1:B:908:MET:HG2	3:B:3241:HOH:O	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:845:ARG:O	1:A:849:ILE:HG13	2.12	0.50
1:A:723:GLU:OE2	1:A:906:PRO:HB2	2.11	0.50
1:B:744:ILE:HG12	3:B:3100:HOH:O	2.10	0.50
1:B:811:LEU:HD13	3:B:3113:HOH:O	2.10	0.50
1:A:880:LEU:O	1:A:884:VAL:HG23	2.12	0.50
1:A:720:GLN:OE1	1:A:724:ARG:NE	2.25	0.49
1:B:919:LYS:HG3	1:B:924:MET:HB2	1.95	0.49
1:A:683:LEU:HA	3:A:3102:HOH:O	2.12	0.49
1:B:800:THR:O	1:B:883:LEU:HD11	2.13	0.48
1:A:725:GLN:O	1:A:729:VAL:HG23	2.13	0.48
1:B:876:LEU:O	1:B:880:LEU:HG	2.13	0.48
1:A:913:ILE:O	1:A:917:LEU:HB2	2.14	0.48
1:B:845:ARG:O	1:B:849:ILE:HG13	2.14	0.48
1:A:886:GLN:HG2	3:A:3137:HOH:O	2.14	0.47
1:B:886:GLN:HA	3:B:3349:HOH:O	2.13	0.47
1:B:804:ILE:N	1:B:805:PRO:HD2	2.30	0.47
1:B:822:LYS:HD2	3:B:3258:HOH:O	2.15	0.47
1:A:721:LEU:CD2	2:A:1001:NOG:HC21	2.44	0.47
1:A:722:GLY:O	1:A:759:MET:HE1	2.15	0.46
1:A:810:LYS:HB2	3:A:3154:HOH:O	2.15	0.46
1:B:733:SER:HB2	1:B:739:PHE:CD2	2.50	0.46
1:B:867:SER:HB2	3:B:3225:HOH:O	2.15	0.46
1:B:730:VAL:O	1:B:734:LYS:HG3	2.16	0.46
1:B:762:GLY:C	1:B:766:ARG:NH2	2.48	0.45
1:A:860:GLN:OE1	1:A:869:ARG:HD2	2.17	0.45
1:A:891:CYS:HB2	2:A:1001:NOG:H162	1.99	0.44
1:A:685:PRO:HA	1:A:686:PRO:HD3	1.83	0.44
1:B:852:LEU:O	1:B:856:ILE:HG13	2.17	0.44
1:B:775:MET:HG2	1:B:785:ASN:HA	1.99	0.44
1:A:723:GLU:CD	1:A:906:PRO:HB2	2.37	0.44
1:A:734:LYS:HG2	3:A:3327:HOH:O	2.16	0.44
1:A:860:GLN:HA	1:A:860:GLN:HE21	1.83	0.43
1:A:725:GLN:OE1	1:A:759:MET:HG2	2.19	0.43
1:A:804:ILE:HD11	1:A:880:LEU:HD21	2.00	0.43
1:B:816:GLU:CD	1:B:816:GLU:H	2.23	0.42
1:B:771:VAL:C	1:B:773:GLY:H	2.22	0.42
1:B:685:PRO:HA	1:B:686:PRO:HD3	1.92	0.42
1:B:872:GLN:HG3	3:B:3113:HOH:O	2.18	0.42
1:B:689:ASN:HB3	3:B:3162:HOH:O	2.20	0.42
1:B:805:PRO:O	1:B:808:PHE:HB2	2.20	0.41
1:A:913:ILE:HG23	1:A:917:LEU:HD12	2.03	0.41
1:B:807:GLU:OE2	1:B:810:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:720:GLN:O	1:B:724:ARG:HG3	2.19	0.41
1:B:730:VAL:HG12	1:B:734:LYS:HE2	2.03	0.41
1:B:878:ASP:OD2	1:B:929:LEU:HA	2.21	0.41
1:B:756:MET:HB3	3:B:3059:HOH:O	2.21	0.41
1:A:931:HIS:HB2	3:A:3284:HOH:O	2.20	0.41
1:B:881:HIS:CD2	1:B:927:PRO:HB3	2.56	0.40
1:A:743:HIS:HD2	1:A:745:ASP:H	1.69	0.40
1:B:763:LEU:HA	1:B:766:ARG:NH2	2.36	0.40
1:A:718:LEU:HB3	2:A:1001:NOG:H112	2.04	0.40
1:B:792:SER:O	1:B:793:SER:CB	2.65	0.40
1:A:805:PRO:HD3	3:A:3285:HOH:O	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	241/258 (93%)	231 (96%)	10 (4%)	0	100	100
1	B	245/258 (95%)	229 (94%)	15 (6%)	1 (0%)	43	46
All	All	486/516 (94%)	460 (95%)	25 (5%)	1 (0%)	56	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	771	VAL

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	225/240 (94%)	222 (99%)	3 (1%)	80	88
1	B	223/240 (93%)	213 (96%)	10 (4%)	38	42
All	All	448/480 (93%)	435 (97%)	13 (3%)	55	64

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	705	ASN
1	A	802	TRP
1	A	815	GLN
1	B	714	LEU
1	B	727	LEU
1	B	728	SER
1	B	766	ARG
1	B	786	GLU
1	B	800	THR
1	B	807	GLU
1	B	840	GLN
1	B	917	LEU
1	B	929	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	689	ASN
1	A	705	ASN
1	A	741	ASN
1	A	743	HIS
1	A	747	GLN
1	A	803	GLN
1	A	812	GLN
1	A	868	GLN
1	A	888	HIS
1	A	897	GLN
1	B	689	ASN
1	B	741	ASN
1	B	840	GLN
1	B	881	HIS
1	B	888	HIS
1	B	897	GLN

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	NOG	A	1001	-	26,26,26	6.47	18 (69%)	41,41,41	3.41	24 (58%)
2	NOG	B	2001	-	26,26,26	6.15	15 (57%)	41,41,41	3.44	25 (60%)

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	NOG	A	1001	-	-	0/3/63/63	0/0/4/4
2	NOG	B	2001	-	-	0/3/63/63	0/0/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NOG	C20-C21	21.44	1.53	1.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	NOG	C20-C21	19.21	1.49	1.18
2	B	2001	NOG	O17-C17	-11.91	1.28	1.43
2	A	1001	NOG	C12-C13	10.36	1.72	1.53
2	B	2001	NOG	C17-C20	9.80	1.60	1.48
2	A	1001	NOG	O17-C17	-8.97	1.32	1.43
2	A	1001	NOG	C9-C8	8.83	1.69	1.54
2	B	2001	NOG	C2-C3	7.94	1.67	1.49
2	A	1001	NOG	C17-C20	7.68	1.57	1.48
2	A	1001	NOG	C2-C3	7.48	1.66	1.49
2	B	2001	NOG	C18-C13	6.78	1.66	1.56
2	B	2001	NOG	C10-C5	6.66	1.63	1.52
2	A	1001	NOG	C16-C17	6.66	1.65	1.55
2	B	2001	NOG	C9-C8	6.29	1.65	1.54
2	B	2001	NOG	C12-C13	6.27	1.64	1.53
2	B	2001	NOG	C1-C10	6.15	1.65	1.53
2	A	1001	NOG	C1-C10	5.84	1.64	1.53
2	A	1001	NOG	C18-C13	5.62	1.64	1.56
2	B	2001	NOG	C4-C5	5.51	1.44	1.34
2	A	1001	NOG	C4-C5	5.00	1.43	1.34
2	A	1001	NOG	C13-C14	4.94	1.64	1.54
2	A	1001	NOG	C10-C5	4.71	1.60	1.52
2	A	1001	NOG	C7-C8	4.20	1.61	1.53
2	B	2001	NOG	C13-C14	4.05	1.62	1.54
2	B	2001	NOG	C13-C17	3.81	1.64	1.56
2	B	2001	NOG	C19-C18	3.56	1.67	1.51
2	A	1001	NOG	C6-C5	3.49	1.60	1.50
2	B	2001	NOG	C7-C8	3.48	1.60	1.53
2	A	1001	NOG	C13-C17	3.39	1.63	1.56
2	B	2001	NOG	C11-C9	3.33	1.59	1.53
2	A	1001	NOG	C8-C14	2.30	1.58	1.53
2	A	1001	NOG	C19-C18	2.30	1.62	1.51
2	A	1001	NOG	C11-C9	2.19	1.57	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	NOG	C12-C13-C17	10.25	121.22	116.55
2	A	1001	NOG	O17-C17-C20	-6.63	100.34	108.58
2	A	1001	NOG	C15-C14-C8	5.91	128.42	119.03
2	A	1001	NOG	C18-C13-C14	-5.88	107.85	111.85
2	B	2001	NOG	C11-C9-C10	5.83	119.21	111.84
2	A	1001	NOG	C18-C13-C17	5.55	112.63	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NOG	C16-C17-C20	5.34	117.17	110.13
2	A	1001	NOG	C12-C13-C17	5.22	118.92	116.55
2	A	1001	NOG	O3-C3-C4	-5.10	113.62	121.59
2	B	2001	NOG	O3-C3-C4	-4.88	113.96	121.59
2	B	2001	NOG	C15-C14-C13	4.88	107.57	104.07
2	B	2001	NOG	C2-C3-C4	4.80	124.09	116.76
2	B	2001	NOG	C15-C14-C8	4.71	126.51	119.03
2	B	2001	NOG	C9-C8-C14	4.71	117.68	109.56
2	A	1001	NOG	C13-C17-C20	-4.47	107.09	111.65
2	B	2001	NOG	C5-C4-C3	-4.47	115.84	123.03
2	A	1001	NOG	C2-C3-C4	4.44	123.54	116.76
2	A	1001	NOG	C10-C9-C8	4.42	117.27	111.86
2	A	1001	NOG	C15-C14-C13	4.30	107.15	104.07
2	A	1001	NOG	C5-C4-C3	-4.24	116.21	123.03
2	B	2001	NOG	C7-C6-C5	4.19	119.61	112.30
2	A	1001	NOG	C9-C8-C14	4.17	116.76	109.56
2	B	2001	NOG	C18-C13-C17	4.15	111.57	108.42
2	A	1001	NOG	C7-C6-C5	4.08	119.42	112.30
2	B	2001	NOG	C16-C17-C20	-4.00	104.86	110.13
2	B	2001	NOG	C18-C13-C12	-3.96	105.52	111.35
2	A	1001	NOG	C11-C9-C10	3.95	116.83	111.84
2	B	2001	NOG	C6-C5-C4	-3.77	113.92	121.47
2	B	2001	NOG	C17-C20-C21	-3.75	171.93	177.06
2	A	1001	NOG	C6-C5-C4	-3.73	114.02	121.47
2	B	2001	NOG	C10-C9-C8	3.60	116.27	111.86
2	A	1001	NOG	C10-C5-C4	3.59	126.85	122.52
2	A	1001	NOG	C11-C9-C8	3.38	117.98	111.14
2	B	2001	NOG	C10-C5-C4	3.31	126.50	122.52
2	B	2001	NOG	C18-C13-C14	-3.29	109.61	111.85
2	B	2001	NOG	C6-C7-C8	3.22	117.09	111.71
2	B	2001	NOG	C13-C14-C8	3.14	117.35	114.23
2	B	2001	NOG	C15-C16-C17	3.07	109.06	106.58
2	A	1001	NOG	C7-C8-C14	2.83	116.83	112.00
2	B	2001	NOG	C11-C9-C8	2.82	116.84	111.14
2	A	1001	NOG	C11-C12-C13	2.82	120.11	112.32
2	A	1001	NOG	C17-C20-C21	-2.70	173.37	177.06
2	B	2001	NOG	C6-C5-C10	2.52	119.52	115.69
2	B	2001	NOG	C7-C8-C14	2.52	116.28	112.00
2	A	1001	NOG	C18-C13-C12	-2.44	107.76	111.35
2	B	2001	NOG	C1-C10-C9	2.38	117.80	111.90
2	A	1001	NOG	C1-C10-C9	2.25	117.49	111.90
2	A	1001	NOG	C6-C5-C10	2.24	119.09	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	2001	NOG	C7-C8-C9	2.06	115.30	111.14

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	247/258 (95%)	-0.34	0 100 100	21, 32, 52, 66	0
1	B	249/258 (96%)	0.11	7 (2%) 50 57	24, 48, 72, 82	0
All	All	496/516 (96%)	-0.12	7 (1%) 72 79	21, 38, 68, 82	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	860	GLN	4.0
1	B	863	VAL	3.1
1	B	849	ILE	2.9
1	B	804	ILE	2.7
1	B	686	PRO	2.6
1	B	806	GLN	2.1
1	B	862	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(\AA^2)	Q<0.9
2	NOG	B	2001	23/23	0.13	0.77	26,30,32,36	0
2	NOG	A	1001	23/23	0.12	0.14	25,27,29,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.