



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2AQU
Title : Structure of HIV-1 protease bound to atazanavir
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Deposited on : 2005-08-18
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

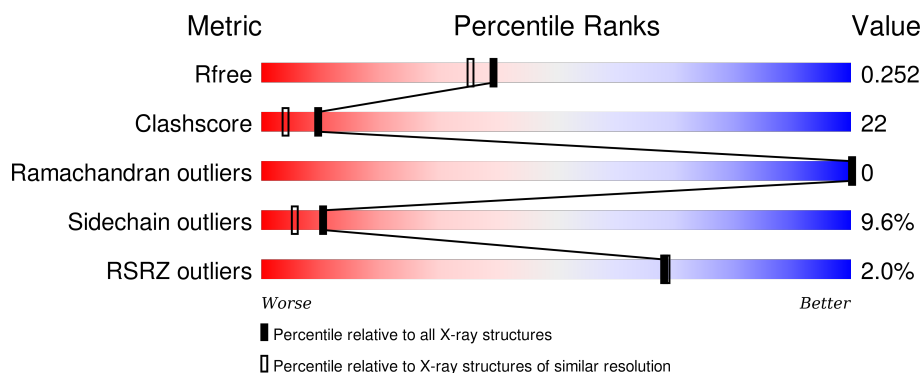
1 Overall quality at a glance

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.

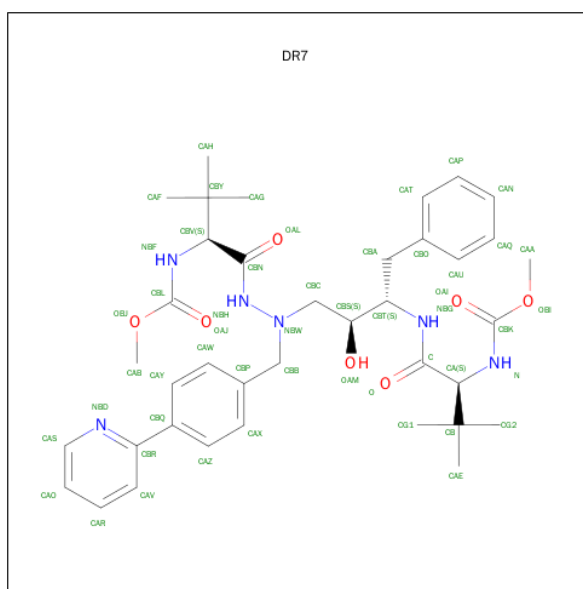
Mol	Chain	Length	Quality of chain
1	A	99	
1	B	99	

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 HIV-1 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total 758	C 489	N 130	O 135	S 4	0	0	0
1	B	99	Total 783	C 507	N 134	O 138	S 4	0	3	0

- Molecule 2 is (3S,8S,9S,12S)-3,12-BIS(1,1-DIMETHYLETHYL)-8-HYDROXY-4,11-DIOXO-9-(PHENYLMETHYL)-6-[[4-(2-PYRIDINYL)PHENYL]METHYL]-2,5,6,10,13-PENTAAZATETRADECANEDIOIC ACID DIMETHYL ESTER (three-letter code: DR7) (formula: C₃₈H₅₂N₆O₇).

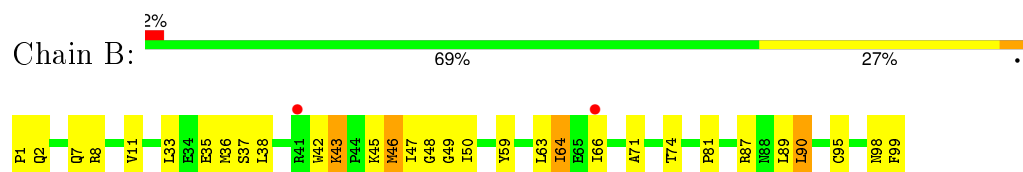


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			102	76	12	14		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	39	Total 39	O 39	0	0

- Molecule 1: HIV-1 Protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	62.41Å 62.41Å 82.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.83 – 2.00 19.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.83-2.00) 94.4 (19.83-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.238 0.241 , 0.252	Depositor DCC
R_{free} test set	595 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.5	EDS
Estimated twinning fraction	0.486 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 12320 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1720	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DR7

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	0.83	0/771	1.02	0/1043
1	B	0.80	0/796	1.05	0/1077
All	All	0.81	0/1567	1.03	0/2120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	758	0	806	44	0
1	B	783	0	839	42	0
2	B	102	0	101	6	0
3	A	38	0	0	2	0
3	B	39	0	0	2	0
All	All	1720	0	1746	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (76) 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:A:59:TYR:HB3	1:A:62:ILE:HD11	1.36	1.07
1:B:33:LEU:HD13	1:B:36:MET:HE1	1.45	0.95
1:A:34:GLU:HG2	1:A:83:ASN:OD1	1.69	0.93
1:A:98:ASN:HD21	1:B:2:GLN:HE21	1.06	0.92
1:B:33:LEU:HD12	1:B:36:MET:HE3	1.52	0.90
1:A:11:VAL:HG21	1:A:67:CYS:HB2	1.55	0.89
1:A:59:TYR:HB3	1:A:62:ILE:CD1	2.04	0.87
1:A:36:MET:HE2	1:A:38:LEU:HD23	1.57	0.87
1:B:33:LEU:CD1	1:B:36:MET:CE	2.53	0.86
1:B:64[A]:ILE:HD13	1:B:71:ALA:O	1.79	0.82
1:B:33:LEU:HD13	1:B:36:MET:CE	2.12	0.80
1:B:45:LYS:CE	1:B:47[B]:ILE:HD11	2.12	0.79
1:A:11:VAL:CG2	1:A:67:CYS:HB2	2.15	0.76
1:B:33:LEU:CD1	1:B:36:MET:HE1	2.15	0.73
1:B:33:LEU:CD1	1:B:36:MET:HE3	2.18	0.73
1:B:45:LYS:HE3	1:B:47[B]:ILE:HD11	1.72	0.70
1:B:45:LYS:HE2	1:B:47[B]:ILE:HD11	1.73	0.69
1:B:33:LEU:HD12	1:B:36:MET:CE	2.18	0.69
1:A:50:ILE:HG22	1:B:49:GLY:HA3	1.73	0.68
1:A:98:ASN:ND2	1:B:2:GLN:HE21	1.88	0.68
1:A:59:TYR:CB	1:A:62:ILE:CD1	2.73	0.66
1:B:7:GLN:HG3	3:B:317:HOH:O	1.98	0.63
1:B:45:LYS:HE3	1:B:47[B]:ILE:CD1	2.30	0.60
1:A:76:LEU:N	1:A:76:LEU:HD12	2.16	0.60
1:A:49:GLY:HA3	1:B:50:ILE:HG22	1.85	0.59
1:A:36:MET:CE	1:A:38:LEU:HD23	2.31	0.59
1:A:98:ASN:HD21	1:B:2:GLN:NE2	1.90	0.58
1:A:15:ILE:HD13	1:A:36:MET:HE1	1.87	0.57
1:A:41:ARG:CG	1:A:41:ARG:HH11	2.18	0.56
1:A:61:GLN:HG3	1:A:72:ILE:HG21	1.88	0.55
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.73	0.53
1:B:64[B]:ILE:HG12	1:B:66:ILE:HG13	1.91	0.53
1:A:31:THR:O	1:A:76:LEU:HD13	2.08	0.53
1:B:64[B]:ILE:HG21	1:B:89:LEU:HD13	1.90	0.52
1:B:64[A]:ILE:H	1:B:64[A]:ILE:HD13	1.74	0.52
1:B:81:PRO:HG2	2:B:300[B]:DR7:CAV	2.41	0.51
1:A:98:ASN:O	1:B:95:CYS:HA	2.11	0.51
1:A:76:LEU:CD1	3:A:102:HOH:O	2.59	0.50
1:B:42:TRP:C	1:B:43[A]:LYS:HG2	2.30	0.50
1:B:47[B]:ILE:CG2	1:B:48:GLY:N	2.75	0.50
1:A:41:ARG:NH1	1:A:41:ARG:CG	2.72	0.50
1:B:46:MET:O	1:B:47[B]:ILE:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:HG2	2:B:300[A]:DR7:CAV	2.42	0.49
1:B:46:MET:C	1:B:47[B]:ILE:HD12	2.33	0.49
1:A:64:ILE:HG21	1:A:89:LEU:HD13	1.95	0.48
1:B:87:ARG:HA	1:B:90:LEU:HB2	1.96	0.48
2:B:300[A]:DR7:HAZ	2:B:300[A]:DR7:HAV	1.57	0.48
1:A:1:PRO:N	1:B:99:PHE:O	2.46	0.47
1:B:64[A]:ILE:N	1:B:64[A]:ILE:HD13	2.29	0.47
1:A:20:LYS:HE3	1:A:36:MET:SD	2.54	0.47
1:A:50:ILE:O	1:A:50:ILE:HG22	2.13	0.47
1:A:2:GLN:HG3	1:B:98:ASN:ND2	2.31	0.45
1:A:99:PHE:O	1:B:1:PRO:N	2.49	0.45
1:A:96:THR:HG21	1:B:2:GLN:NE2	2.32	0.45
1:A:36:MET:HE2	1:A:38:LEU:CD2	2.39	0.45
1:B:59:TYR:O	1:B:74:THR:HA	2.16	0.45
1:B:43[B]:LYS:HE3	1:B:43[B]:LYS:HB3	1.55	0.45
1:A:40:GLY:HA3	3:A:129:HOH:O	2.17	0.45
1:A:4:THR:CG2	1:A:6:TRP:HD1	2.30	0.44
1:A:63:LEU:HD22	1:A:64:ILE:N	2.32	0.44
1:A:45:LYS:CG	1:A:46:MET:N	2.80	0.44
1:B:36:MET:SD	1:B:38:LEU:HD21	2.58	0.44
1:A:95:CYS:HA	1:B:98:ASN:O	2.18	0.43
2:B:300[A]:DR7:O	2:B:300[A]:DR7:HAE2	2.19	0.43
1:A:76:LEU:CD1	1:A:76:LEU:N	2.79	0.43
1:B:49:GLY:HA2	2:B:300[A]:DR7:CAZ	2.49	0.43
1:B:35:GLU:HB2	3:B:338:HOH:O	2.19	0.43
1:A:61:GLN:HG3	1:A:72:ILE:CG2	2.48	0.42
2:B:300[B]:DR7:HAV	2:B:300[B]:DR7:HAZ	1.43	0.42
1:A:29:ASP:OD2	1:B:8:ARG:NH2	2.49	0.42
1:A:50:ILE:O	1:A:50:ILE:CG2	2.67	0.41
1:A:96:THR:HG22	1:B:98:ASN:HB2	2.02	0.41
1:A:42:TRP:N	1:A:42:TRP:CD1	2.87	0.41
1:A:56:VAL:HG21	1:A:76:LEU:HD23	2.03	0.41
1:A:36:MET:CE	1:A:38:LEU:CD2	2.98	0.40
1:B:64[A]:ILE:HG13	1:B:89:LEU:HD13	2.04	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	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
1	B	100/99 (101%)	100 (100%)	0	0	100	100
All	All	197/198 (100%)	196 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/83 (100%)	74 (89%)	9 (11%)	8	4
1	B	86/83 (104%)	77 (90%)	9 (10%)	8	4
All	All	169/166 (102%)	151 (89%)	18 (11%)	10	4

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	37	SER
1	A	38	LEU
1	A	41	ARG
1	A	50	ILE
1	A	62	ILE
1	A	63	LEU
1	A	79	PRO

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Mol	Chain	Res	Type
1	A	96	THR
1	B	11	VAL
1	B	37	SER
1	B	43[A]	LYS
1	B	43[B]	LYS
1	B	46	MET
1	B	63	LEU
1	B	64[A]	ILE
1	B	64[B]	ILE
1	B	90	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	DR7	B	300[A]	-	52,53,53	2.78	17 (32%)	68,74,74	4.25	28 (41%)
2	DR7	B	300[B]	-	52,53,53	2.40	15 (28%)	68,74,74	3.95	26 (38%)

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	DR7	B	300[A]	-	-	0/59/60/60	0/3/3/3
2	DR7	B	300[B]	-	-	0/59/60/60	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300[B]	DR7	CBQ-CBR	-8.36	1.36	1.48
2	B	300[A]	DR7	CBQ-CBR	-6.72	1.38	1.48
2	B	300[A]	DR7	CBC-CBS	-6.20	1.42	1.52
2	B	300[A]	DR7	CB-CA	-5.33	1.46	1.55
2	B	300[B]	DR7	CBC-CBS	-4.76	1.45	1.52
2	B	300[B]	DR7	O-C	-3.95	1.15	1.23
2	B	300[A]	DR7	OAL-CBN	-3.81	1.15	1.23
2	B	300[B]	DR7	OAL-CBN	-3.60	1.16	1.23
2	B	300[A]	DR7	CG2-CB	-3.28	1.46	1.53
2	B	300[B]	DR7	OAM-CBS	-3.20	1.36	1.43
2	B	300[A]	DR7	O-C	-3.18	1.17	1.23
2	B	300[B]	DR7	CAZ-CAX	-3.06	1.33	1.38
2	B	300[B]	DR7	OBI-CAA	-2.85	1.38	1.45
2	B	300[B]	DR7	CBC-NBW	-2.71	1.43	1.48
2	B	300[A]	DR7	CBC-NBW	-2.68	1.44	1.48
2	B	300[B]	DR7	CBA-CBT	-2.56	1.48	1.53
2	B	300[B]	DR7	OAJ-CBL	-2.51	1.16	1.21
2	B	300[A]	DR7	OBI-CAA	-2.36	1.39	1.45
2	B	300[B]	DR7	CG2-CB	-2.35	1.48	1.53
2	B	300[A]	DR7	OAM-CBS	-2.33	1.38	1.43
2	B	300[B]	DR7	CB-CA	-2.29	1.52	1.55
2	B	300[A]	DR7	OAJ-CBL	-2.25	1.17	1.21
2	B	300[A]	DR7	CBA-CBT	-2.15	1.49	1.53
2	B	300[A]	DR7	OBJ-CAB	-2.04	1.40	1.45
2	B	300[A]	DR7	CAV-CBR	2.20	1.44	1.38
2	B	300[B]	DR7	NBH-NBW	3.56	1.44	1.41
2	B	300[B]	DR7	OBJ-CBL	4.93	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300[A]	DR7	OBI-CBK	5.70	1.42	1.34
2	B	300[B]	DR7	OBI-CBK	5.99	1.42	1.34
2	B	300[A]	DR7	OBJ-CBL	6.03	1.42	1.34
2	B	300[A]	DR7	CBK-N	6.33	1.51	1.34
2	B	300[A]	DR7	CA-C	8.79	1.70	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300[A]	DR7	CB-CA-C	-10.01	102.71	112.83
2	B	300[A]	DR7	C-CA-N	-9.56	88.51	108.94
2	B	300[A]	DR7	OAM-CBS-CBC	-7.41	92.94	110.45
2	B	300[B]	DR7	OAM-CBS-CBC	-7.18	93.49	110.45
2	B	300[A]	DR7	CBA-CBT-NBG	-5.63	103.98	110.14
2	B	300[B]	DR7	OBJ-CBL-OAJ	-5.61	117.39	124.70
2	B	300[B]	DR7	CAZ-CBQ-CBR	-5.07	112.98	121.24
2	B	300[A]	DR7	OBI-CBK-OAI	-5.05	118.11	124.70
2	B	300[A]	DR7	OBJ-CBL-OAJ	-4.94	118.26	124.70
2	B	300[B]	DR7	CBA-CBT-NBG	-4.84	104.85	110.14
2	B	300[A]	DR7	CG2-CB-CA	-4.39	100.64	109.75
2	B	300[A]	DR7	CAV-CBR-NBD	-4.27	115.77	122.28
2	B	300[B]	DR7	CAV-CBR-NBD	-4.13	115.97	122.28
2	B	300[A]	DR7	CAZ-CBQ-CBR	-3.98	114.75	121.24
2	B	300[B]	DR7	CBB-CBP-CAX	-3.30	114.55	120.78
2	B	300[A]	DR7	CBB-CBP-CAX	-2.92	115.26	120.78
2	B	300[B]	DR7	OBI-CBK-OAI	-2.87	120.96	124.70
2	B	300[A]	DR7	CA-C-NBG	-2.40	112.07	115.46
2	B	300[B]	DR7	CAW-CAY-CBQ	-2.15	118.00	121.14
2	B	300[B]	DR7	CAO-CAR-CAV	-2.15	117.04	120.19
2	B	300[A]	DR7	CAS-NBD-CBR	2.09	120.08	117.20
2	B	300[B]	DR7	CAS-NBD-CBR	2.11	120.10	117.20
2	B	300[A]	DR7	CG1-CB-CA	2.20	114.31	109.75
2	B	300[B]	DR7	CAB-OBJ-CBL	2.26	118.42	115.63
2	B	300[B]	DR7	OBI-CBK-N	2.34	115.03	110.64
2	B	300[B]	DR7	CBB-CBP-CAW	2.36	125.23	120.78
2	B	300[A]	DR7	CBB-CBP-CAW	2.41	125.33	120.78
2	B	300[A]	DR7	CAB-OBJ-CBL	2.45	118.66	115.63
2	B	300[A]	DR7	OAM-CBS-CBT	2.45	114.87	109.21
2	B	300[A]	DR7	CAE-CB-CA	2.55	115.03	109.75
2	B	300[B]	DR7	OAM-CBS-CBT	2.61	115.23	109.21
2	B	300[A]	DR7	OBJ-CBL-NBF	2.78	115.86	110.64
2	B	300[B]	DR7	CBT-NBG-C	2.88	128.48	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300[B]	DR7	OBJ-CBL-NBF	2.95	116.16	110.64
2	B	300[A]	DR7	CAY-CBQ-CBR	2.97	126.09	121.24
2	B	300[A]	DR7	OBI-CBK-N	3.06	116.38	110.64
2	B	300[B]	DR7	CAA-OBI-CBK	3.34	119.77	115.63
2	B	300[B]	DR7	CAY-CBQ-CBR	3.35	126.71	121.24
2	B	300[A]	DR7	CAR-CAV-CBR	3.64	123.75	118.88
2	B	300[B]	DR7	CB-CA-C	3.68	116.55	112.83
2	B	300[A]	DR7	CBT-NBG-C	3.73	130.07	123.13
2	B	300[A]	DR7	CBQ-CBR-NBD	3.95	124.87	116.78
2	B	300[B]	DR7	CAR-CAV-CBR	4.09	124.34	118.88
2	B	300[B]	DR7	CBQ-CBR-NBD	4.36	125.70	116.78
2	B	300[A]	DR7	CBY-CBV-CBN	4.61	117.48	112.83
2	B	300[B]	DR7	CBY-CBV-CBN	4.63	117.50	112.83
2	B	300[A]	DR7	CBS-CBT-NBG	4.65	117.22	109.73
2	B	300[B]	DR7	CBS-CBT-NBG	5.10	117.94	109.73
2	B	300[A]	DR7	CBB-NBW-NBH	6.46	117.44	109.74
2	B	300[B]	DR7	CBB-NBW-NBH	8.31	119.65	109.74
2	B	300[B]	DR7	CBC-NBW-NBH	10.52	125.17	110.18
2	B	300[A]	DR7	CBC-NBW-NBH	11.32	126.31	110.18
2	B	300[A]	DR7	CBN-NBH-NBW	21.77	142.57	120.29
2	B	300[B]	DR7	CBN-NBH-NBW	22.40	143.22	120.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	300[A]	DR7	4	0
2	B	300[B]	DR7	2	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	99/99 (100%)	-0.22	2 (2%) 68 69	13, 28, 43, 61	1 (1%)
1	B	99/99 (100%)	-0.24	2 (2%) 68 69	18, 28, 44, 56	0
All	All	198/198 (100%)	-0.23	4 (2%) 68 69	13, 28, 44, 61	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	ILE	3.7
1	A	15	ILE	3.7
1	A	41	ARG	2.5
1	B	41	ARG	2.4

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
2	DR7	B	300[A]	51/51	0.94	0.13	1.18	20,26,38,38	51
2	DR7	B	300[B]	51/51	0.94	0.13	1.18	22,27,36,37	51

6.5 Other polymers [i](#)

There are no such residues in this entry.