



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:49 pm GMT

PDB ID : 2NLL
Title : RETINOID X RECEPTOR-THYROID HORMONE RECEPTOR DNA-BINDING DOMAIN HETERODIMER BOUND TO THYROID RESPONSE ELEMENT DNA
Authors : Rastinejad, F.; Perlmann, T.; Evans, R.M.; Sigler, P.B.
Deposited on : 1996-11-20
Resolution : 1.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

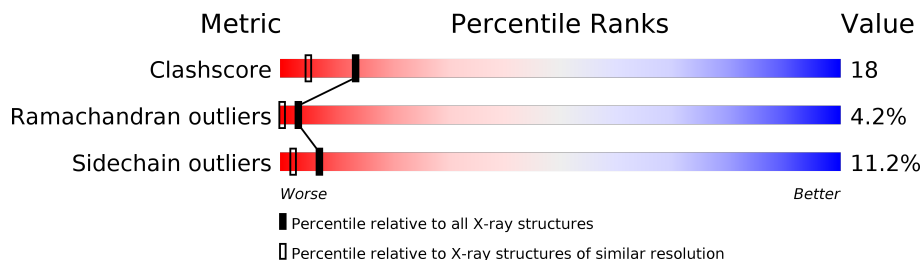
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	18	
2	D	18	
3	A	66	
4	B	103	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2351 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*AP*GP*GP*TP*CP*AP*TP*TP*(5IU)P*CP*AP*GP*GP*TP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	18	Total	C	I	N	O	P	0	0	0
			367	175	1	67	107	17			

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*GP*AP*CP*CP*TP*GP*AP*AP*AP*TP*GP*AP*CP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	P	0	0	0
			365	175	68	105	17			

- Molecule 3 is a protein called PROTEIN (RETINOIC ACID RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	66	Total	C	N	O	S	0	0	0
			533	323	104	95	11			

- Molecule 4 is a protein called PROTEIN (THYROID HORMONE RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	103	Total	C	N	O	S	0	0	0
			846	521	159	155	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	401	GLU	GLN	CONFLICT	UNP P10828

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	A	2	Total 2	Zn 2	0	0

- Molecule 6 is water.

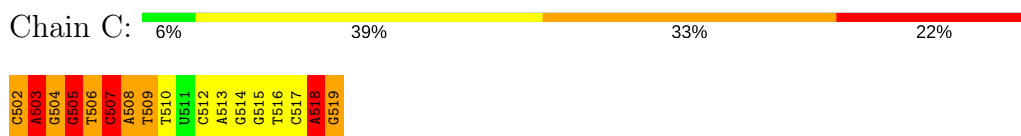
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total 52	O 52	0	0
6	B	83	Total 83	O 83	0	0
6	C	58	Total 58	O 58	0	0
6	D	43	Total 43	O 43	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

Note EDS was not executed.

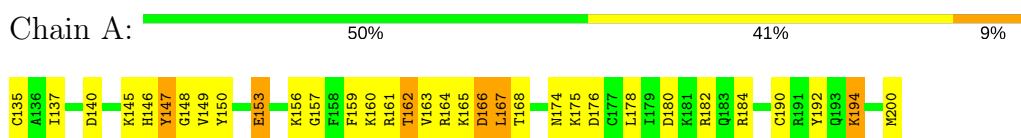
- Molecule 1: DNA (5'-D(*CP*AP*GP*GP*TP*CP*AP*TP*TP*(5IU)P*CP*AP*GP*GP*TP*CP*AP*G)-3')



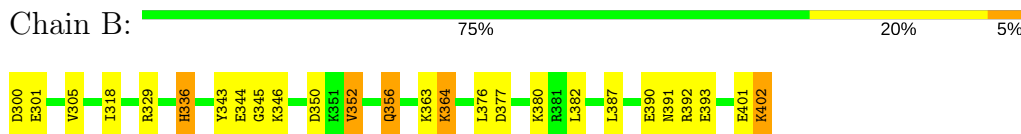
- Molecule 2: DNA (5'-D(*CP*TP*GP*AP*CP*CP*TP*GP*AP*AP*AP*TP*GP*AP*CP*CP*T P*G)-3')



- Molecule 3: PROTEIN (RETINOIC ACID RECEPTOR)



- Molecule 4: PROTEIN (THYROID HORMONE RECEPTOR)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.90 Å 65.60 Å 125.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	87.0 (6.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2351	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5IU

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	C	3.06	40/388 (10.3%)	2.35	31/595 (5.2%)
2	D	2.90	33/409 (8.1%)	2.58	43/629 (6.8%)
3	A	0.52	0/540	0.70	0/713
4	B	0.67	0/856	0.84	0/1136
All	All	1.86	73/2193 (3.3%)	1.68	74/3073 (2.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
2	D	0	5
All	All	0	9

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	524	DA	N9-C4	14.38	1.46	1.37
1	C	504	DG	P-O5'	13.23	1.73	1.59
1	C	503	DA	P-O5'	12.52	1.72	1.59
1	C	504	DG	O3'-P	11.71	1.75	1.61
1	C	516	DT	C5-C7	-10.33	1.43	1.50
2	D	531	DA	N9-C4	10.12	1.44	1.37
2	D	524	DA	P-O5'	9.78	1.69	1.59
1	C	513	DA	P-O5'	9.70	1.69	1.59
1	C	503	DA	O3'-P	9.00	1.72	1.61
2	D	537	DT	N1-C2	8.91	1.45	1.38
2	D	527	DT	O3'-P	-8.49	1.50	1.61
1	C	509	DT	P-O5'	8.48	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	DA	N9-C4	8.46	1.43	1.37
1	C	515	DG	O3'-P	-8.39	1.51	1.61
2	D	530	DA	C5-C4	-8.04	1.33	1.38
2	D	526	DC	C2-N3	7.96	1.42	1.35
2	D	524	DA	C6-N1	-7.85	1.30	1.35
2	D	522	DT	C5-C7	7.71	1.54	1.50
1	C	504	DG	C3'-O3'	7.60	1.53	1.44
1	C	508	DA	O4'-C1'	7.51	1.51	1.42
2	D	531	DA	C6-N6	-7.41	1.28	1.33
1	C	514	DG	O3'-P	7.21	1.69	1.61
2	D	522	DT	P-O5'	-7.11	1.52	1.59
1	C	510	DT	N1-C2	7.07	1.43	1.38
1	C	504	DG	C8-N7	7.05	1.35	1.30
1	C	505	DG	O3'-P	7.03	1.69	1.61
1	C	507	DC	P-O5'	6.99	1.66	1.59
2	D	532	DT	O3'-P	6.94	1.69	1.61
1	C	506	DT	C5-C7	6.92	1.54	1.50
2	D	527	DT	C5-C7	6.91	1.54	1.50
1	C	515	DG	O4'-C1'	6.84	1.50	1.42
1	C	516	DT	P-O5'	6.81	1.66	1.59
2	D	526	DC	C5-C6	6.75	1.39	1.34
2	D	537	DT	P-O5'	6.59	1.66	1.59
2	D	523	DG	O3'-P	-6.58	1.53	1.61
1	C	509	DT	C5-C7	6.54	1.53	1.50
1	C	509	DT	O3'-P	-6.43	1.53	1.61
2	D	527	DT	C4-C5	6.33	1.50	1.45
1	C	517	DC	P-O5'	-6.24	1.53	1.59
2	D	526	DC	N1-C2	-6.19	1.33	1.40
2	D	529	DA	P-O5'	6.17	1.66	1.59
2	D	530	DA	N1-C2	-6.03	1.28	1.34
1	C	508	DA	C6-N1	-6.03	1.31	1.35
2	D	525	DC	C4-C5	6.00	1.47	1.43
1	C	509	DT	C4-C5	-5.98	1.39	1.45
2	D	532	DT	N1-C6	-5.98	1.34	1.38
2	D	532	DT	C5-C7	5.96	1.53	1.50
2	D	537	DT	C2-O2	5.95	1.27	1.22
1	C	505	DG	O4'-C1'	5.93	1.49	1.42
1	C	513	DA	C4'-C3'	-5.81	1.46	1.52
2	D	526	DC	C3'-O3'	-5.75	1.36	1.44
1	C	514	DG	C4'-C3'	-5.73	1.46	1.52
1	C	502	DC	C3'-O3'	-5.63	1.36	1.44
1	C	515	DG	C2-N3	5.59	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	510	DT	C5-C7	5.56	1.53	1.50
2	D	533	DG	N1-C2	5.56	1.42	1.37
1	C	518	DA	O3'-P	5.54	1.67	1.61
1	C	506	DT	N3-C4	-5.43	1.34	1.38
2	D	524	DA	C5-C6	5.38	1.45	1.41
1	C	506	DT	C2-N3	-5.37	1.33	1.37
1	C	515	DG	N3-C4	5.36	1.39	1.35
1	C	502	DC	N3-C4	5.33	1.37	1.33
1	C	503	DA	N3-C4	5.24	1.38	1.34
1	C	510	DT	C4-O4	-5.24	1.18	1.23
2	D	522	DT	N1-C6	-5.17	1.34	1.38
1	C	518	DA	O4'-C1'	5.14	1.48	1.42
2	D	528	DG	N9-C8	-5.11	1.34	1.37
1	C	510	DT	O4'-C1'	5.09	1.48	1.42
2	D	538	DG	N3-C4	-5.08	1.31	1.35
2	D	528	DG	N7-C5	-5.08	1.36	1.39
2	D	526	DC	O3'-P	-5.07	1.55	1.61
2	D	522	DT	N3-C4	-5.06	1.34	1.38
1	C	509	DT	O4'-C1'	5.03	1.48	1.42

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	521	DC	P-O3'-C3'	19.60	143.22	119.70
1	C	509	DT	P-O3'-C3'	15.71	138.55	119.70
2	D	530	DA	P-O3'-C3'	12.30	134.46	119.70
2	D	529	DA	P-O3'-C3'	12.04	134.14	119.70
1	C	518	DA	P-O3'-C3'	11.35	133.32	119.70
2	D	523	DG	P-O3'-C3'	10.30	132.07	119.70
1	C	507	DC	P-O3'-C3'	10.24	131.99	119.70
1	C	517	DC	P-O3'-C3'	10.21	131.95	119.70
1	C	506	DT	P-O3'-C3'	-9.78	107.97	119.70
2	D	525	DC	P-O3'-C3'	9.32	130.88	119.70
2	D	535	DC	P-O3'-C3'	8.90	130.38	119.70
1	C	503	DA	P-O3'-C3'	8.84	130.30	119.70
2	D	532	DT	P-O3'-C3'	8.47	129.87	119.70
2	D	522	DT	P-O3'-C3'	8.28	129.64	119.70
2	D	533	DG	C5-C6-O6	-8.14	123.72	128.60
2	D	527	DT	P-O3'-C3'	8.01	129.31	119.70
1	C	513	DA	P-O3'-C3'	7.64	128.87	119.70
2	D	532	DT	N1-C2-N3	7.46	119.08	114.60
2	D	527	DT	C6-C5-C7	-7.35	118.49	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	531	DA	P-O3'-C3'	7.28	128.44	119.70
1	C	506	DT	C4'-C3'-C2'	7.27	109.64	103.10
1	C	519	DG	N1-C6-O6	-7.18	115.59	119.90
2	D	522	DT	N1-C2-N3	7.12	118.87	114.60
2	D	537	DT	C4-C5-C6	7.00	122.20	118.00
1	C	519	DG	C5-C6-O6	6.93	132.76	128.60
2	D	522	DT	N3-C2-O2	-6.83	118.20	122.30
1	C	516	DT	C4-C5-C6	6.71	122.03	118.00
2	D	526	DC	P-O3'-C3'	6.70	127.74	119.70
2	D	524	DA	C5-N7-C8	6.59	107.20	103.90
2	D	532	DT	N3-C2-O2	-6.52	118.39	122.30
2	D	524	DA	P-O3'-C3'	6.47	127.46	119.70
2	D	533	DG	N1-C6-O6	6.38	123.73	119.90
1	C	506	DT	C5-C6-N1	-6.37	119.88	123.70
1	C	515	DG	C4'-C3'-C2'	6.17	108.65	103.10
2	D	522	DT	C4-C5-C6	6.17	121.70	118.00
1	C	508	DA	P-O3'-C3'	6.10	127.02	119.70
1	C	502	DC	C4'-C3'-C2'	6.08	108.57	103.10
1	C	512	DC	C2-N3-C4	6.07	122.93	119.90
2	D	532	DT	C4-C5-C6	6.06	121.64	118.00
2	D	527	DT	C4-C5-C6	6.06	121.64	118.00
1	C	509	DT	C4'-C3'-C2'	6.05	108.54	103.10
1	C	514	DG	P-O3'-C3'	6.01	126.91	119.70
1	C	509	DT	C4-C5-C6	5.98	121.59	118.00
1	C	510	DT	C4-C5-C6	5.93	121.56	118.00
2	D	526	DC	N3-C4-C5	-5.92	119.53	121.90
1	C	516	DT	C4'-C3'-C2'	5.84	108.36	103.10
2	D	525	DC	C4'-C3'-C2'	5.79	108.31	103.10
2	D	526	DC	C6-N1-C2	5.77	122.61	120.30
2	D	536	DC	P-O3'-C3'	5.75	126.60	119.70
2	D	527	DT	N1-C2-N3	5.73	118.04	114.60
1	C	506	DT	N1-C2-N3	5.70	118.02	114.60
2	D	531	DA	C4'-C3'-C2'	5.66	108.19	103.10
2	D	534	DA	C4'-C3'-C2'	5.65	108.19	103.10
1	C	508	DA	C4'-C3'-C2'	5.62	108.16	103.10
2	D	532	DT	C5-C6-N1	-5.60	120.34	123.70
1	C	510	DT	C5-C6-N1	-5.54	120.38	123.70
2	D	535	DC	C2-N3-C4	5.41	122.60	119.90
1	C	502	DC	C2-N3-C4	5.35	122.58	119.90
1	C	518	DA	C4'-C3'-C2'	5.33	107.89	103.10
2	D	526	DC	C2-N3-C4	5.29	122.54	119.90
2	D	526	DC	C2-N1-C1'	-5.27	113.00	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	533	DG	C3'-C2'-C1'	-5.25	96.20	102.50
2	D	537	DT	C4'-C3'-C2'	5.22	107.80	103.10
2	D	535	DC	N3-C4-C5	-5.22	119.81	121.90
1	C	515	DG	P-O3'-C3'	5.21	125.95	119.70
2	D	536	DC	C4'-C3'-C2'	5.19	107.77	103.10
1	C	505	DG	N1-C6-O6	-5.15	116.81	119.90
1	C	502	DC	N3-C4-C5	-5.07	119.87	121.90
1	C	504	DG	C8-N9-C4	-5.07	104.37	106.40
2	D	527	DT	C4'-C3'-C2'	5.04	107.63	103.10
2	D	529	DA	C4'-C3'-C2'	5.02	107.62	103.10
1	C	514	DG	C4'-C3'-C2'	5.01	107.61	103.10
2	D	532	DT	C4'-C3'-C2'	5.00	107.60	103.10
2	D	535	DC	C4'-C3'-C2'	5.00	107.60	103.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	503	DA	Sidechain
1	C	505	DG	Sidechain
1	C	507	DC	Sidechain
1	C	518	DA	Sidechain
2	D	524	DA	Sidechain
2	D	529	DA	Sidechain
2	D	531	DA	Sidechain
2	D	533	DG	Sidechain
2	D	538	DG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	367	0	202	15	0
2	D	365	0	202	8	0
3	A	533	0	518	31	0
4	B	846	0	850	20	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
6	A	52	0	0	3	0
6	B	83	0	0	1	0
6	C	58	0	0	0	0
6	D	43	0	0	0	0
All	All	2351	0	1772	68	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 18.

All (68) 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)
3:A:175:LYS:HD2	3:A:190:CYS:SG	2.00	1.01
3:A:159:PHE:HB3	6:A:838:HOH:O	1.73	0.89
3:A:157:GLY:HA2	3:A:160:LYS:HE3	1.54	0.87
3:A:148:GLY:HA3	3:A:200:MET:HA	1.56	0.87
4:B:377:ASP:H	4:B:380:LYS:HZ3	1.22	0.84
3:A:137:ILE:HG23	3:A:194:LYS:HD2	1.68	0.75
4:B:336:HIS:H	4:B:336:HIS:CD2	2.05	0.74
3:A:175:LYS:HA	3:A:190:CYS:SG	2.27	0.73
4:B:402:LYS:HA	4:B:402:LYS:NZ	2.05	0.71
3:A:190:CYS:O	3:A:194:LYS:HB2	1.94	0.68
1:C:502:DC:H3'	3:A:145:LYS:O	1.94	0.66
3:A:145:LYS:HA	3:A:150:TYR:HA	1.77	0.65
3:A:153:GLU:HA	3:A:156:LYS:HB3	1.78	0.64
4:B:377:ASP:H	4:B:380:LYS:NZ	1.96	0.63
1:C:503:DA:H2''	1:C:504:DG:H5''	1.82	0.61
4:B:343:TYR:CD2	4:B:344:GLU:HG2	2.35	0.60
4:B:401:GLU:O	4:B:402:LYS:HG2	2.02	0.59
3:A:148:GLY:CA	3:A:200:MET:HA	2.30	0.59
1:C:503:DA:H1'	1:C:504:DG:OP1	2.03	0.59
4:B:336:HIS:H	4:B:336:HIS:HD2	1.52	0.58
1:C:506:DT:H2'	1:C:507:DC:C6	2.39	0.57
2:D:526:DC:H2''	2:D:527:DT:O5'	2.05	0.56
2:D:532:DT:OP2	3:A:161:ARG:NH1	2.39	0.56
3:A:157:GLY:O	3:A:161:ARG:HG3	2.06	0.56
4:B:356:GLN:HA	4:B:356:GLN:OE1	2.05	0.56
4:B:305:VAL:HG13	4:B:364:LYS:HG3	1.87	0.55
2:D:535:DC:H2''	2:D:536:DC:C6	2.41	0.55
1:C:503:DA:H1'	1:C:504:DG:P	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:160:LYS:NZ	6:A:756:HOH:O	2.36	0.55
4:B:402:LYS:HA	4:B:402:LYS:HZ2	1.70	0.53
1:C:508:DA:H1'	1:C:509:DT:H5'	1.89	0.53
4:B:391:ASN:C	4:B:393:GLU:H	2.12	0.53
3:A:163:VAL:HA	3:A:166:ASP:OD2	2.10	0.52
4:B:391:ASN:O	4:B:393:GLU:N	2.42	0.52
4:B:390:GLU:O	4:B:393:GLU:HB3	2.10	0.52
3:A:167:LEU:N	6:A:789:HOH:O	2.40	0.51
1:C:505:DG:H2'	1:C:506:DT:C6	2.45	0.51
1:C:503:DA:OP2	3:A:146:HIS:HA	2.11	0.51
3:A:157:GLY:HA2	3:A:160:LYS:CE	2.34	0.51
3:A:165:LYS:HB2	3:A:165:LYS:NZ	2.26	0.50
3:A:159:PHE:CG	3:A:200:MET:SD	3.05	0.50
3:A:140:ASP:HB2	3:A:184:ARG:HH12	1.77	0.50
3:A:153:GLU:HG3	3:A:156:LYS:HD3	1.94	0.49
3:A:162:THR:HG21	3:A:192:TYR:CD1	2.48	0.48
1:C:502:DC:H1'	1:C:503:DA:N7	2.28	0.48
2:D:532:DT:H2'	3:A:161:ARG:NH2	2.29	0.48
4:B:336:HIS:CD2	4:B:336:HIS:N	2.80	0.46
2:D:535:DC:H2''	2:D:536:DC:H6	1.80	0.46
1:C:503:DA:P	3:A:146:HIS:HA	2.55	0.46
2:D:535:DC:H2''	2:D:536:DC:OP2	2.15	0.46
4:B:391:ASN:C	4:B:393:GLU:N	2.70	0.44
1:C:503:DA:H2''	1:C:504:DG:C5'	2.48	0.44
2:D:523:DG:N7	4:B:329:ARG:NH2	2.64	0.44
1:C:518:DA:H2''	1:C:519:DG:O5'	2.17	0.44
3:A:135:CYS:N	3:A:140:ASP:O	2.51	0.43
3:A:175:LYS:HD2	3:A:175:LYS:HA	1.88	0.43
4:B:346:LYS:HG2	6:B:657:HOH:O	2.18	0.43
3:A:147:TYR:CD1	3:A:147:TYR:N	2.82	0.43
4:B:350:ASP:OD1	4:B:352:VAL:HG13	2.18	0.43
4:B:300:ASP:HA	4:B:318:ILE:HD13	2.00	0.43
1:C:505:DG:H2'	1:C:506:DT:H6	1.84	0.43
1:C:507:DC:H6	1:C:507:DC:H2'	1.71	0.43
3:A:175:LYS:CD	3:A:190:CYS:SG	2.89	0.42
3:A:176:ASP:N	3:A:176:ASP:OD1	2.52	0.42
1:C:504:DG:H2''	1:C:505:DG:O4'	2.19	0.42
4:B:402:LYS:HA	4:B:402:LYS:HZ3	1.81	0.41
2:D:534:DA:H2''	2:D:535:DC:C6	2.54	0.41
3:A:167:LEU:HD22	3:A:168:THR:H	1.86	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	64/66 (97%)	48 (75%)	12 (19%)	4 (6%)	1	0
4	B	101/103 (98%)	94 (93%)	4 (4%)	3 (3%)	5	1
All	All	165/169 (98%)	142 (86%)	16 (10%)	7 (4%)	3	0

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	147	TYR
3	A	164	ARG
4	B	301	GLU
4	B	392	ARG
4	B	345	GLY
3	A	162	THR
3	A	149	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	58/58 (100%)	50 (86%)	8 (14%)	4	1
4	B	94/94 (100%)	85 (90%)	9 (10%)	10	3
All	All	152/152 (100%)	135 (89%)	17 (11%)	7	2

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	153	GLU
3	A	166	ASP
3	A	167	LEU
3	A	174	ASN
3	A	178	LEU
3	A	180	ASP
3	A	182	ARG
3	A	194	LYS
4	B	336	HIS
4	B	352	VAL
4	B	356	GLN
4	B	363	LYS
4	B	364	LYS
4	B	376	LEU
4	B	382	LEU
4	B	387	LEU
4	B	402	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	185	ASN
4	B	336	HIS
4	B	355	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	5IU	C	511	1,2	13,21,22	1.25	1 (7%)	15,30,33	3.39	3 (20%)

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
1	5IU	C	511	1,2	-	0/3/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	511	5IU	O3'-C3'	2.61	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	511	5IU	C5-C4-N3	-5.86	115.43	123.27
1	C	511	5IU	C2'-C3'-C4'	2.01	107.01	102.73
1	C	511	5IU	C4-N3-C2	11.27	125.01	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.