



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 10:07 AM EDT

PDB ID : 1YNW  
Title : Crystal Structure of Vitamin D Receptor and 9-cis Retinoic Acid Receptor  
DNA-Binding Domains Bound to a DR3 Response Element  
Authors : Shaffer, P.L.; Gewirth, D.T.  
Deposited on : 2005-01-25  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

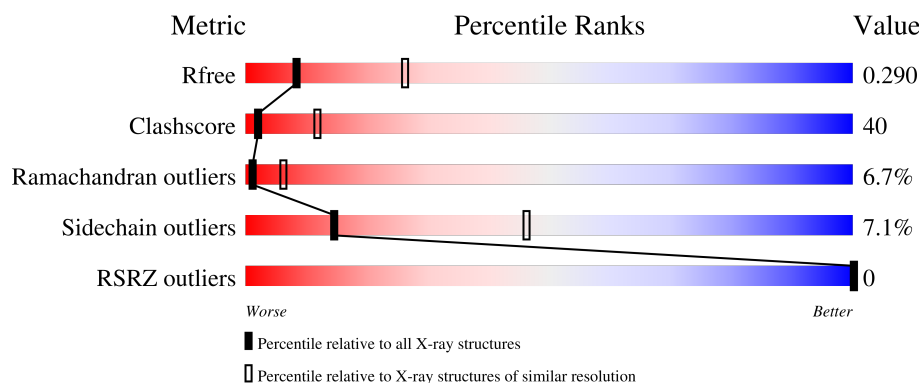
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	C	18	<div> <div>11%</div> <div>78%</div> <div>11%</div> </div>
2	D	18	<div> <div>11%</div> <div>72%</div> <div>17%</div> </div>
3	A	110	<div> <div>34%</div> <div>46%</div> <div>7%</div> <div>13%</div> </div>
4	B	99	<div> <div>39%</div> <div>29%</div> <div>5%</div> <div>26%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2070 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 5'-d(\*TP\*TP\*AP\*GP\*GP\*TP\*CP\*AP\*CP\*GP\*AP\*AP\*GP\*GP\*TP\*CP\*AP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	18	Total	C	N	O	P	0	0	0
			370	177	72	104	17			

- Molecule 2 is a DNA chain called 5'-d(\*TP\*TP\*TP\*GP\*AP\*CP\*CP\*TP\*TP\*CP\*GP\*TP\*GP\*AP\*CP\*CP\*TP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	P	0	0	0
			361	175	59	110	17			

- Molecule 3 is a protein called Vitamin D3 Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	96	Total	C	N	O	S	0	0	0
			761	464	154	129	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	ALA	PRO	engineered mutation	UNP P11473
A	62	ALA	PHE	engineered mutation	UNP P11473
A	75	ALA	HIS	engineered mutation	UNP P11473

- Molecule 4 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	73	Total	C	N	O	S	0	0	0
			574	350	109	104	11			

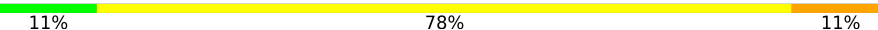
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

### 3 Residue-property plots

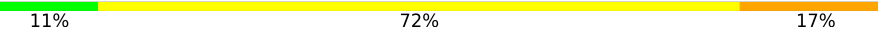
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Molecule 1: 5'-d(\*TP\*TP\*AP\*GP\*GP\*TP\*CP\*AP\*CP\*GP\*AP\*AP\*GP\*GP\*TP\*CP\*AP\*A)-3'

Chain C: 

T401  
T402  
A403  
G404  
G405  
T406  
C407  
A408  
G410  
A411  
A412  
G413  
G414  
A417  
A418

- Molecule 2: 5'-d(\*TP\*TP\*TP\*GP\*AP\*CP\*CP\*TP\*TP\*CP\*GP\*TP\*GP\*AP\*CP\*CP\*TP\*A)-3'

Chain D: 

T419  
T420  
T421  
G422  
A423  
C424  
C425  
T426  
T427  
G428  
G429  
T430  
G431  
A432  
C433  
C434  
T435  
A436

- Molecule 3: Vitamin D3 Receptor

Chain A: 

PHE  
ASP  
R18  
M19  
V20  
P21  
R22  
T23  
C24  
G25  
V26  
C27  
G28  
D29  
R30  
A31  
T32  
G33  
F34  
H35  
F36  
N37  
E42  
G43  
C44  
K45  
G46  
F47  
F48  
R49  
R50  
S51  
M52  
F58  
T59  
C60  
A61  
A62  
N63  
G64  
D65  
C66  
T69  
K70  
D71  
N72  
R73  
R74  
A75  
Q76  
Q77  
A78  
C79  
R80  
M90  
K91

E92  
F93  
I94  
L95  
T96  
D97  
E98  
E99  
V100  
Q101  
R102  
D103  
K104  
R105  
M106  
I107  
L108  
K109  
R110  
K111  
E112  
E113  
GLU  
ALA  
LEU  
LYS  
ASP  
SER  
LEU  
ARG  
PRO  
LYS  
LEU  
SER

- Molecule 4: Retinoic acid receptor RXR-alpha

Chain B: 

PHE  
THR  
LYS  
HIS  
I234  
C235  
A236  
I237  
C238  
G239  
D240  
R241  
H246  
Y247  
G248  
S251  
C252  
E253  
K256  
G257  
F258  
F259  
K260  
R261  
T262  
V263  
R264  
Y269  
I270  
C271  
R272  
D273  
N274  
K275  
L278  
I279  
R284  
Q288  
Y289  
C290  
R291  
Y292  
C295  
L296  
A297  
M298  
G299  
M300  
Q305  
GLU  
GLU

ARG  
GLN  
ARG  
GLY  
LYS  
ASP  
ARG  
ASN  
ASN  
GLU  
GLU  
VAL  
GLU  
SER  
THR  
SER  
SER  
ALA  
ASN  
GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.10Å 57.05Å 73.44Å 90.00° 110.31° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 24.44 – 2.99	Depositor EDS
% Data completeness (in resolution range)	87.6 (50.00-3.00) 90.4 (24.44-2.99)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 2.99Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.283 0.234 , 0.290	Depositor DCC
$R_{free}$ test set	823 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN

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	1.12	0/416	0.97	1/641 (0.2%)
2	D	1.12	0/402	1.02	0/618
3	A	0.74	0/768	0.86	0/1015
4	B	0.65	0/581	0.79	0/772
All	All	0.88	0/2167	0.90	1/3046 (0.0%)

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	2
2	D	0	5
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	403	DA	O5'-P-OP1	5.27	117.03	110.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	401	DT	Sidechain
1	C	412	DA	Sidechain
2	D	419	DT	Sidechain

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Mol	Chain	Res	Type	Group
2	D	423	DA	Sidechain
2	D	425	DC	Sidechain
2	D	430	DT	Sidechain
2	D	436	DA	Sidechain

## 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	C	370	0	204	32	0
2	D	361	0	207	28	0
3	A	761	0	771	69	0
4	B	574	0	551	27	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
All	All	2070	0	1733	152	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 40.

All (152) 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:74:ARG:HH11	3:A:74:ARG:HB3	1.34	0.92
1:C:417:DA:H2''	1:C:418:DA:H5''	1.49	0.91
3:A:35:HIS:ND1	3:A:45:LYS:HD2	1.85	0.88
2:D:426:DT:H2''	2:D:427:DT:H5''	1.58	0.85
4:B:262:THR:HG21	4:B:292:TYR:CD1	2.14	0.82
3:A:111:LYS:O	3:A:113:GLU:HG2	1.82	0.79
4:B:271:CYS:SG	4:B:275:LYS:HA	2.25	0.75
3:A:74:ARG:HB3	3:A:74:ARG:NH1	2.01	0.74
1:C:411:DA:H1'	1:C:412:DA:C8	2.21	0.74
2:D:429:DG:H2''	2:D:430:DT:C5'	2.17	0.74
4:B:271:CYS:HB2	4:B:289:TYR:CD2	2.22	0.74
2:D:426:DT:H2''	2:D:427:DT:C5'	2.18	0.72
3:A:70:LYS:HD3	3:A:70:LYS:C	2.10	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:110:ARG:O	3:A:110:ARG:HG2	1.91	0.70
2:D:426:DT:C2'	2:D:427:DT:H5''	2.21	0.70
1:C:417:DA:C2'	1:C:418:DA:H5''	2.21	0.70
1:C:403:DA:H5''	1:C:403:DA:H8	1.56	0.69
3:A:101:GLN:O	3:A:105:GLU:HG3	1.92	0.69
1:C:413:DG:H2''	1:C:414:DG:H5'	1.74	0.69
2:D:423:DA:H2''	2:D:424:DC:H5'	1.74	0.69
3:A:60:CYS:SG	3:A:64:GLY:HA2	2.33	0.69
2:D:420:DT:H2''	2:D:421:DT:H5'	1.73	0.68
2:D:420:DT:H1'	2:D:421:DT:H5''	1.75	0.68
1:C:403:DA:H2'	1:C:404:DG:C8	2.30	0.67
1:C:402:DT:H2''	1:C:403:DA:H5''	1.77	0.66
3:A:103:LYS:O	3:A:107:ILE:HD13	1.93	0.66
3:A:74:ARG:NH1	3:A:74:ARG:CB	2.58	0.66
3:A:100:VAL:HG12	3:A:104:ARG:HH11	1.61	0.65
1:C:413:DG:H2''	1:C:414:DG:C5'	2.27	0.64
3:A:27:CYS:SG	3:A:29:ASP:HB2	2.37	0.64
3:A:70:LYS:HD3	3:A:70:LYS:O	1.98	0.64
3:A:47:PHE:CD2	3:A:80:ARG:HD3	2.33	0.64
1:C:408:DA:H1'	1:C:409:DC:H5''	1.79	0.63
1:C:409:DC:H2''	1:C:410:DG:O5'	1.99	0.63
2:D:420:DT:H2''	2:D:421:DT:C5'	2.28	0.62
2:D:429:DG:H2''	2:D:430:DT:H5'	1.81	0.61
1:C:411:DA:C4	1:C:412:DA:N7	2.68	0.61
2:D:419:DT:H4'	2:D:420:DT:OP1	1.98	0.61
1:C:412:DA:H2''	1:C:413:DG:O5'	2.01	0.61
2:D:432:DA:H2''	2:D:433:DC:H5'	1.82	0.60
1:C:408:DA:OP2	1:C:408:DA:H8	1.85	0.60
3:A:35:HIS:CE1	3:A:45:LYS:HD2	2.37	0.60
4:B:292:TYR:CE2	4:B:296:LEU:HD11	2.37	0.60
2:D:429:DG:H1'	2:D:430:DT:H5''	1.82	0.59
4:B:262:THR:HG21	4:B:292:TYR:CE1	2.37	0.59
1:C:410:DG:H2'	1:C:411:DA:C8	2.38	0.59
4:B:240:ASP:OD2	4:B:241:ARG:N	2.35	0.58
4:B:258:PHE:CD2	4:B:291:ARG:HD3	2.39	0.58
3:A:112:GLU:O	3:A:112:GLU:HG3	2.02	0.58
3:A:48:PHE:O	3:A:52:MET:HG2	2.03	0.57
1:C:410:DG:H4'	1:C:410:DG:OP1	2.05	0.57
3:A:108:LEU:CD1	3:A:111:LYS:HD3	2.35	0.57
2:D:419:DT:H2''	2:D:420:DT:C7	2.35	0.57
3:A:36:PHE:HE2	3:A:45:LYS:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:73:ARG:HG3	3:A:74:ARG:H	1.70	0.56
2:D:419:DT:H2''	2:D:420:DT:H72	1.89	0.55
3:A:107:ILE:HD12	3:A:107:ILE:N	2.21	0.55
1:C:405:DG:H1'	1:C:406:DT:H5''	1.87	0.55
3:A:58:PHE:HB2	3:A:78:ALA:HA	1.87	0.55
1:C:405:DG:H2''	1:C:406:DT:C5'	2.36	0.55
3:A:49:ARG:HH21	3:A:49:ARG:HB2	1.71	0.55
2:D:429:DG:H2''	2:D:430:DT:H5''	1.88	0.55
4:B:235:CYS:SG	4:B:251:SER:HA	2.47	0.55
3:A:49:ARG:HH21	3:A:49:ARG:CB	2.21	0.54
2:D:423:DA:H2''	2:D:424:DC:C5'	2.36	0.54
1:C:405:DG:H2''	1:C:406:DT:H5'	1.89	0.54
2:D:427:DT:H5'	2:D:427:DT:H6	1.73	0.54
3:A:18:ARG:O	3:A:18:ARG:HG3	2.08	0.54
3:A:74:ARG:HH11	3:A:74:ARG:CB	2.11	0.53
1:C:402:DT:H2''	1:C:403:DA:C8	2.44	0.53
2:D:431:DG:H5''	3:A:73:ARG:HH21	1.73	0.53
3:A:35:HIS:O	3:A:36:PHE:C	2.48	0.53
3:A:101:GLN:HA	3:A:104:ARG:NH1	2.24	0.52
3:A:29:ASP:OD2	3:A:30:ARG:N	2.40	0.52
3:A:22:ARG:NH1	3:A:33:GLY:HA2	2.25	0.52
3:A:102:ARG:NH2	3:A:103:LYS:NZ	2.58	0.52
4:B:246:HIS:O	4:B:247:TYR:C	2.47	0.51
3:A:108:LEU:HD12	3:A:111:LYS:HD3	1.91	0.51
4:B:271:CYS:SG	4:B:290:CYS:SG	3.08	0.51
4:B:237:ILE:HD13	4:B:298:MET:HG3	1.93	0.51
3:A:45:LYS:HG2	3:A:46:GLY:N	2.26	0.50
3:A:32:THR:OG1	3:A:42:GLU:HG2	2.11	0.50
4:B:279:ILE:HD12	4:B:284:ARG:HA	1.94	0.50
3:A:49:ARG:CB	3:A:49:ARG:NH2	2.75	0.50
3:A:77:GLN:O	3:A:78:ALA:C	2.49	0.50
3:A:100:VAL:HG12	3:A:104:ARG:NH1	2.26	0.50
3:A:61:ALA:O	3:A:62:ALA:O	2.30	0.49
4:B:239:GLY:O	4:B:240:ASP:O	2.31	0.49
1:C:402:DT:H2''	1:C:403:DA:H8	1.76	0.49
2:D:419:DT:C2'	2:D:420:DT:H72	2.43	0.48
1:C:403:DA:H5''	1:C:403:DA:C8	2.44	0.48
3:A:96:THR:O	3:A:100:VAL:HG23	2.14	0.48
4:B:292:TYR:O	4:B:295:CYS:HB2	2.13	0.48
3:A:107:ILE:N	3:A:107:ILE:CD1	2.76	0.47
3:A:69:THR:N	3:A:72:ASN:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:73:ARG:HG3	3:A:74:ARG:N	2.28	0.47
4:B:246:HIS:O	4:B:248:GLY:N	2.47	0.47
2:D:431:DG:OP2	3:A:80:ARG:NH1	2.45	0.47
2:D:420:DT:C1'	2:D:421:DT:H5''	2.43	0.47
4:B:258:PHE:CE2	4:B:291:ARG:HG2	2.50	0.46
3:A:49:ARG:O	3:A:50:ARG:C	2.54	0.46
4:B:260:LYS:O	4:B:261:ARG:C	2.53	0.46
4:B:271:CYS:SG	4:B:275:LYS:CA	3.02	0.46
1:C:411:DA:H1'	1:C:412:DA:H8	1.76	0.46
4:B:269:TYR:CD2	4:B:288:GLN:HB3	2.52	0.45
1:C:404:DG:C2	1:C:405:DG:C5	3.05	0.45
4:B:274:ASN:O	4:B:275:LYS:HB2	2.16	0.45
1:C:410:DG:H2''	1:C:411:DA:O5'	2.16	0.45
3:A:27:CYS:SG	3:A:29:ASP:CB	3.05	0.45
4:B:253:GLU:O	4:B:256:LYS:HB3	2.16	0.44
1:C:408:DA:OP2	1:C:408:DA:C8	2.68	0.44
2:D:420:DT:C2'	2:D:421:DT:C5'	2.95	0.44
4:B:272:ARG:HG3	4:B:272:ARG:O	2.18	0.43
1:C:406:DT:H2''	1:C:407:DC:H5'	1.99	0.43
3:A:72:ASN:O	3:A:73:ARG:C	2.57	0.43
4:B:269:TYR:CD2	4:B:288:GLN:OE1	2.71	0.43
2:D:423:DA:H1'	2:D:424:DC:H5''	2.00	0.43
2:D:429:DG:C2'	2:D:430:DT:H5''	2.47	0.43
3:A:108:LEU:O	3:A:111:LYS:HB3	2.18	0.43
2:D:434:DC:H2''	2:D:435:DT:H72	2.00	0.43
3:A:73:ARG:CG	3:A:74:ARG:H	2.31	0.43
3:A:102:ARG:HH21	3:A:103:LYS:NZ	2.16	0.43
3:A:18:ARG:O	3:A:19:ASN:HB2	2.19	0.43
3:A:24:CYS:SG	3:A:26:VAL:HB	2.59	0.43
3:A:60:CYS:SG	3:A:64:GLY:CA	3.03	0.43
3:A:35:HIS:O	3:A:37:ASN:N	2.52	0.42
3:A:36:PHE:CD2	3:A:36:PHE:N	2.88	0.42
3:A:47:PHE:CE2	3:A:80:ARG:HD3	2.54	0.42
3:A:73:ARG:O	3:A:75:ALA:N	2.52	0.42
4:B:258:PHE:CZ	4:B:292:TYR:HB2	2.54	0.42
3:A:26:VAL:HG11	3:A:44:CYS:SG	2.59	0.42
3:A:47:PHE:CD2	3:A:80:ARG:CD	3.02	0.42
1:C:413:DG:OP1	4:B:264:ARG:NH2	2.40	0.42
3:A:109:LYS:C	3:A:111:LYS:H	2.23	0.42
2:D:431:DG:H5''	3:A:73:ARG:NH2	2.35	0.42
3:A:60:CYS:SG	3:A:64:GLY:N	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:74:ARG:CB	3:A:74:ARG:CZ	2.97	0.41
3:A:74:ARG:NH1	3:A:74:ARG:HB2	2.35	0.41
3:A:108:LEU:HD12	3:A:108:LEU:O	2.21	0.41
1:C:411:DA:H2''	1:C:412:DA:OP2	2.20	0.41
3:A:22:ARG:O	3:A:31:ALA:N	2.46	0.41
3:A:74:ARG:CZ	3:A:74:ARG:HB2	2.51	0.41
4:B:279:ILE:HD13	4:B:279:ILE:HA	1.79	0.41
1:C:410:DG:H2''	1:C:411:DA:C5'	2.51	0.41
3:A:36:PHE:CE1	3:A:94:ILE:HG12	2.55	0.41
1:C:411:DA:C6	1:C:412:DA:N6	2.89	0.40
4:B:259:PHE:CE2	4:B:300:MET:HB3	2.56	0.40
1:C:408:DA:OP2	1:C:408:DA:H2'	2.21	0.40
1:C:406:DT:H5'	1:C:406:DT:H6	1.86	0.40
2:D:420:DT:C2'	2:D:421:DT:H5''	2.51	0.40
2:D:429:DG:C1'	2:D:430:DT:H5''	2.50	0.40
3:A:107:ILE:CD1	3:A:107:ILE:H	2.35	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	
3	A	94/110 (86%)	63 (67%)	23 (24%)	8 (8%)	1	4
4	B	71/99 (72%)	55 (78%)	13 (18%)	3 (4%)	3	16
All	All	165/209 (79%)	118 (72%)	36 (22%)	11 (7%)	1	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	62	ALA
4	B	240	ASP

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Mol	Chain	Res	Type
4	B	247	TYR
3	A	73	ARG
3	A	74	ARG
3	A	112	GLU
3	A	65	ASP
3	A	98	GLU
4	B	264	ARG
3	A	36	PHE
3	A	21	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	
3	A	80/95 (84%)	73 (91%)	7 (9%)	10	36
4	B	61/88 (69%)	58 (95%)	3 (5%)	25	61
All	All	141/183 (77%)	131 (93%)	10 (7%)	14	46

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	VAL
3	A	60	CYS
3	A	66	CYS
3	A	70	LYS
3	A	90	MET
3	A	92	GLU
3	A	109	LYS
4	B	241	ARG
4	B	272	ARG
4	B	278	LEU

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

Mol	Chain	Res	Type
3	A	37	ASN

### 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 monosaccharides 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	18/18 (100%)	-0.51	0 100 100	77, 94, 107, 111	0
2	D	18/18 (100%)	-0.50	0 100 100	72, 96, 107, 112	0
3	A	96/110 (87%)	-0.23	0 100 100	81, 104, 120, 127	0
4	B	73/99 (73%)	-0.10	0 100 100	92, 105, 121, 123	0
All	All	205/245 (83%)	-0.23	0 100 100	72, 102, 120, 127	0

There are no RSRZ outliers to report.

### 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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	ZN	B	351	1/1	0.90	0.11	129,129,129,129	0
5	ZN	A	150	1/1	0.98	0.19	92,92,92,92	0
5	ZN	B	350	1/1	0.99	0.24	99,99,99,99	0
5	ZN	A	151	1/1	0.99	0.12	120,120,120,120	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.