



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:13 PM UTC

PDB ID : 1YNW / pdb_00001ynw
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

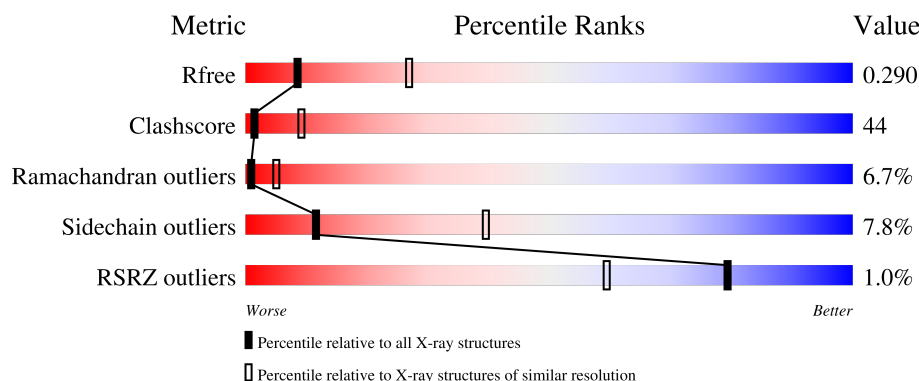
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 ≥ 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	
2	D	18	
3	A	110	
4	B	99	

2 Entry composition

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			

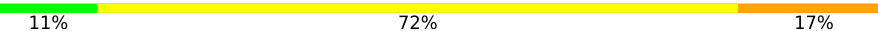
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

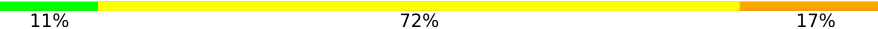
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

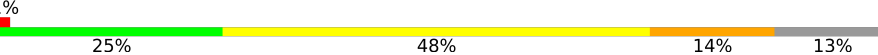
T401
T402
A403
G404
G405
T406
C407
A408
C409
G410
A411
A412
G413
G414
A417
A418

- 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
C429
G430
T431
A432
C433
C434
T435
A436

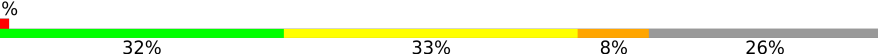
- Molecule 3: Vitamin D3 Receptor

Chain A: 

PHE
ASP
R18
M19
V20
P21
R22
T23
C24
G25
V26
C27
G28
D29
R30
A31
T32
G33
F34
H35
F36
N37
A38
T39
T40
C41
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
C76
Q77
C79
R80

D86
I87
G88
M89
M90
I94
L95
T96
D97
E98
E99
V100
Q101
R102
K103
R104
E105
M106
I107
L108
K109
R110
K111
E112
E113
GLU
ALA
LEU
LYS
ASP
LEU
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
S242
H246
Y247
G248
V249
Y250
S251
C252
E253
K256
G257
F258
F259
K260
R261
T262
V263
R264
R265
D266
Y269
T270
C271
R272
D273
N274
K275
L276
I279
R284
Q288
Y289
C290
R291
Y292
Q293
K294
C295
L296
A297
N298
G299

K300
G306
GLU
GLU
ARG
GLN
ARG
GLY
LYS
ASP
ARG
ASN
GLU
ASN
GLU
VAL
SER
THR
SER
ALA
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.10Å 57.05Å 73.44Å 90.00° 110.31° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.6 (50.00-3.00) 87.2 (50.00-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	96.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.70	0/416	1.00	2/641 (0.3%)
2	D	0.67	0/402	0.97	0/618
3	A	0.88	1/768 (0.1%)	1.26	9/1015 (0.9%)
4	B	0.71	0/581	1.05	2/772 (0.3%)
All	All	0.76	1/2167 (0.0%)	1.10	13/3046 (0.4%)

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	2
2	D	0	5
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	106	MET	SD-CE	6.48	1.95	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	111	LYS	N-CA-C	-11.56	98.70	113.72
3	A	37	ASN	N-CA-C	8.59	123.06	112.58
3	A	97	ASP	N-CA-C	-8.55	102.04	111.36
3	A	88	GLY	N-CA-C	6.53	124.32	115.32
1	C	403	DA	C4'-C3'-O3'	6.05	119.08	110.00
3	A	27	CYS	N-CA-C	6.02	119.93	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	249	VAL	N-CA-C	5.86	116.30	108.27
3	A	71	ASP	N-CA-C	5.79	120.36	113.12
3	A	40	THR	N-CA-C	5.61	117.71	109.24
3	A	20	VAL	CA-C-N	5.52	126.74	119.84
3	A	20	VAL	C-N-CA	5.52	126.74	119.84
4	B	284	ARG	N-CA-C	-5.47	106.65	113.38
1	C	418	DA	C4'-C3'-O3'	-5.44	101.84	110.00

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
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	27	0
3	A	761	0	771	76	0
4	B	574	0	551	33	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
All	All	2070	0	1733	164	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 44.

All (164) 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)
2:D:419:DT:H2''	2:D:420:DT:H71	1.40	1.00
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
3:A:35:HIS:HD1	3:A:45:LYS:HD2	1.49	0.77
3:A:70:LYS:HD3	3:A:70:LYS:C	2.10	0.76
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
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
3:A:110:ARG:O	3:A:110:ARG:HG2	1.91	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
2:D:419:DT:C2'	2:D:420:DT:H71	2.20	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
4:B:236:ALA:HB1	4:B:298:MET:HE2	1.78	0.65
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
3:A:48:PHE:CD2	3:A:89:MET:HE2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:HIS:O	3:A:36:PHE:C	2.48	0.57
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
3:A:36:PHE:HE2	3:A:45:LYS:HG3	1.70	0.56
3:A:73:ARG:HG3	3:A:74:ARG:H	1.70	0.56
4:B:246:HIS:O	4:B:247:TYR:C	2.47	0.56
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
3:A:77:GLN:O	3:A:78:ALA:C	2.49	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: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
3:A:108:LEU:HD12	3:A:111:LYS:HD3	1.91	0.51
3:A:49:ARG:O	3:A:50:ARG:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:260:LYS:O	4:B:261:ARG:C	2.53	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: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
1:C:403:DA:H5''	1:C:403:DA:C8	2.44	0.48
3:A:72:ASN:O	3:A:73:ARG:C	2.57	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
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
3:A:109:LYS:C	3:A:111:LYS:H	2.23	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
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
3:A:100:VAL:O	3:A:101:GLN:C	2.60	0.44
4:B:253:GLU:O	4:B:256:LYS:HB3	2.16	0.44
4:B:291:ARG:O	4:B:292:TYR:C	2.59	0.44
1:C:408:DA:OP2	1:C:408:DA:C8	2.68	0.44
4:B:294:LYS:O	4:B:295:CYS:C	2.60	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:108:LEU:O	3:A:111:LYS:HB3	2.18	0.43
4:B:266:ASP:O	4:B:266:ASP:CG	2.61	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:34:PHE:CE2	3:A:39:MET:HE2	2.54	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
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
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
4:B:249:VAL:O	4:B:250:TYR:C	2.60	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:103:LYS:O	3:A:104:ARG:C	2.63	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:234:ILE:C	4:B:242:SER:HB2	2.46	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:86:ASP:C	3:A:88:GLY:H	2.29	0.40
3:A:98:GLU:O	3:A:99:GLU:C	2.64	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%)	0	3
4	B	71/99 (72%)	55 (78%)	13 (18%)	3 (4%)	2	13
All	All	165/209 (79%)	118 (72%)	36 (22%)	11 (7%)	1	5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	62	ALA
4	B	240	ASP
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%)	9	35
4	B	61/88 (69%)	57 (93%)	4 (7%)	15	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	141/183 (77%)	130 (92%)	11 (8%)	11	39

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	VAL
3	A	26	VAL
3	A	60	CYS
3	A	66	CYS
3	A	70	LYS
3	A	90	MET
3	A	109	LYS
4	B	241	ARG
4	B	272	ARG
4	B	278	LEU
4	B	279	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	35	HIS
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 oligosaccharides 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, 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	C	18/18 (100%)	0.46	0	100 100	77, 94, 107, 111	0
2	D	18/18 (100%)	0.21	0	100 100	72, 96, 107, 112	0
3	A	96/110 (87%)	0.03	1 (1%)	79 59	81, 104, 120, 127	0
4	B	73/99 (73%)	0.16	1 (1%)	73 51	92, 105, 121, 123	0
All	All	205/245 (83%)	0.13	2 (0%)	79 59	72, 102, 120, 127	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	248	GLY	2.4
3	A	90	MET	2.1

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	B	350	1/1	0.97	0.10	99,99,99,99	0
5	ZN	A	150	1/1	0.98	0.07	92,92,92,92	0
5	ZN	B	351	1/1	0.98	0.06	129,129,129,129	0
5	ZN	A	151	1/1	1.00	0.04	120,120,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.