



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:29 AM UTC

PDB ID : 1OUP / pdb_00001oup
Title : Crystal structure of the periplasmic endonuclease Vvn complexed with octamer double stranded DNA
Authors : Yuan, H.S.; Li, C.-L.
Deposited on : 2003-03-25
Resolution : 2.30 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

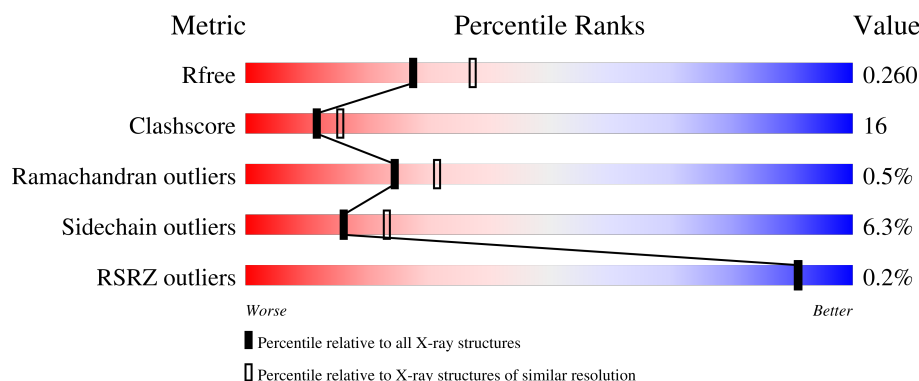
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	8	88%12%
1	D	8	38%62%
1	F	8	38%38%25%
2	E	6	17%67%17%
3	G	2	100%

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Mol	Chain	Length	Quality of chain
4	A	213	74% 24%
4	B	213	63% 30% 6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4425 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(*GP*CP*GP*AP*TP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	8	Total	C	N	O	P	0	0	0
			161	77	31	46	7			
1	D	8	Total	C	N	O	P	0	0	0
			161	77	31	46	7			
1	F	8	Total	C	N	O	P	0	0	0
			161	77	31	46	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	P	0	0	0
			120	58	23	34	5			

- Molecule 3 is a DNA chain called 5'-D(P*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	P	0	0	0
			42	19	8	13	2			

- Molecule 4 is a protein called Nuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	213	Total	C	N	O	S	0	0	0
			1738	1080	324	321	13			
4	B	210	Total	C	N	O	S	0	0	0
			1712	1066	319	314	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	ALA	HIS	engineered mutation	UNP Q8DCA6
A	163	PRO	GLN	SEE REMARK 999	UNP Q8DCA6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	164	ASP	THR	SEE REMARK 999	UNP Q8DCA6
A	165	ARG	GLU	SEE REMARK 999	UNP Q8DCA6
A	166	ALA	LEU	SEE REMARK 999	UNP Q8DCA6
B	80	ALA	HIS	engineered mutation	UNP Q8DCA6
B	163	PRO	GLN	SEE REMARK 999	UNP Q8DCA6
B	164	ASP	THR	SEE REMARK 999	UNP Q8DCA6
B	165	ARG	GLU	SEE REMARK 999	UNP Q8DCA6
B	166	ALA	LEU	SEE REMARK 999	UNP Q8DCA6

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	9	Total O 9 9	0	0
6	D	4	Total O 4 4	0	0
6	E	3	Total O 3 3	0	0
6	G	3	Total O 3 3	0	0
6	F	8	Total O 8 8	0	0
6	A	188	Total O 188 188	0	0
6	B	113	Total O 113 113	0	0

3 Residue-property plots [i](#)

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.

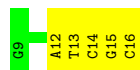
- Molecule 1: 5'-D(*GP*CP*GP*AP*TP*CP*GP*C)-3'

Chain C:  88% 12%



- Molecule 1: 5'-D(*GP*CP*GP*AP*TP*CP*GP*C)-3'

Chain D:  38% 62%

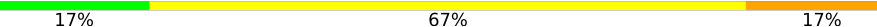


- Molecule 1: 5'-D(*GP*CP*GP*AP*TP*CP*GP*C)-3'

Chain F:  38% 38% 25%



- Molecule 2: 5'-D(*GP*CP*GP*AP*TP*C)-3'

Chain E:  17% 67% 17%



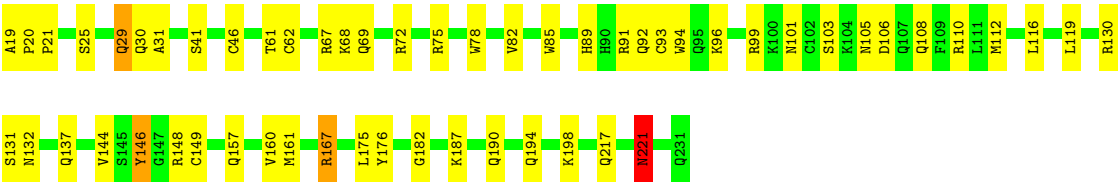
- Molecule 3: 5'-D(P*GP*C)-3'

Chain G:  100%

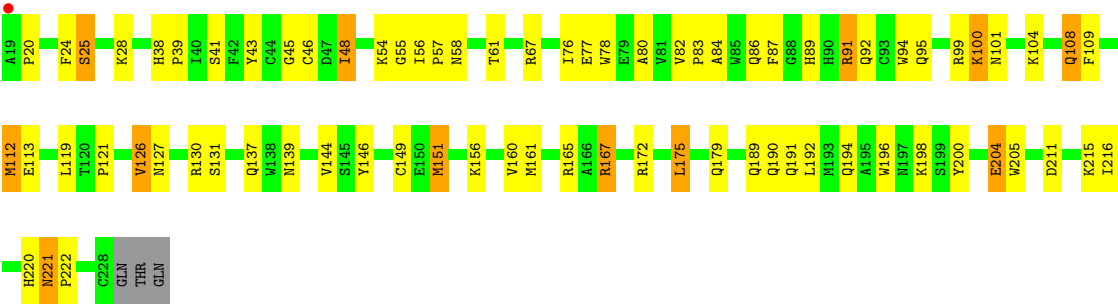


- Molecule 4: Nuclease

Chain A:  74% 24%



• Molecule 4: Nuclease



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.74Å 50.11Å 89.61Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	19.78 – 2.30 19.78 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.78-2.30) 97.4 (19.78-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.191 , 0.260 0.191 , 0.260	Depositor DCC
R_{free} test set	1616 reflections (7.64%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4425	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9519e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.32	0/180	0.61	0/276
1	D	0.34	0/180	0.73	0/276
1	F	0.36	0/180	0.96	0/276
2	E	0.34	0/134	0.69	0/205
3	G	0.74	0/46	1.31	1/67 (1.5%)
4	A	0.71	0/1783	1.03	6/2404 (0.2%)
4	B	0.65	2/1757 (0.1%)	1.00	7/2370 (0.3%)
All	All	0.64	2/4260 (0.0%)	0.98	14/5874 (0.2%)

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	F	0	2
2	E	0	2
3	G	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	131	SER	CA-C	-5.48	1.48	1.53
4	B	112	MET	SD-CE	-5.18	1.66	1.79

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	82	VAL	N-CA-C	-9.71	97.95	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	82	VAL	N-CA-C	-9.65	98.00	107.55
4	B	131	SER	CB-CA-C	-7.58	107.82	116.54
3	G	8	DC	C2'-C3'-O3'	-6.61	101.59	111.50
4	B	91	ARG	N-CA-C	5.98	118.67	110.24
4	A	182	GLY	N-CA-C	5.75	122.78	114.10
4	B	80	ALA	N-CA-C	-5.74	99.17	108.41
4	A	146	TYR	N-CA-C	5.71	117.29	110.44
4	A	119	LEU	N-CA-C	5.45	118.12	109.24
4	A	167	ARG	N-CA-C	5.28	117.72	111.33
4	B	48	ILE	N-CA-C	5.21	115.40	108.11
4	A	221	ASN	N-CA-C	-5.14	99.45	108.69
4	B	126	VAL	N-CA-C	-5.14	105.53	110.72
4	B	167	ARG	N-CA-C	5.03	116.45	111.07

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	4	DA	Sidechain
2	E	5	DT	Sidechain
1	F	11	DG	Sidechain
1	F	13	DT	Sidechain
3	G	7	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	161	0	91	2	0
1	D	161	0	91	4	0
1	F	161	0	91	13	0
2	E	120	0	69	9	0
3	G	42	0	23	5	0
4	A	1738	0	1640	40	0
4	B	1712	0	1617	58	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	188	0	0	5	0
6	B	113	0	0	10	0
6	C	9	0	0	1	0
6	D	4	0	0	0	0
6	E	3	0	0	0	0
6	F	8	0	0	1	0
6	G	3	0	0	0	0
All	All	4425	0	3622	123	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 16.

All (123) 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)
4:B:91:ARG:NH2	4:B:112:MET:HE1	1.64	1.12
4:B:91:ARG:HH22	4:B:112:MET:HE1	1.24	0.92
1:D:15:DG:H2''	1:D:16:DC:H5''	1.50	0.91
4:A:161:MET:HE2	4:A:167:ARG:HH22	1.37	0.89
2:E:1:DG:H2''	2:E:2:DC:H5'	1.54	0.89
4:B:161:MET:HE2	4:B:167:ARG:HH22	1.40	0.84
2:E:6:DC:H2'	3:G:7:DG:OP2	1.78	0.84
4:A:148:ARG:HD3	6:A:672:HOH:O	1.77	0.84
1:F:11:DG:H2''	1:F:12:DA:H5''	1.59	0.83
4:A:198:LYS:HG2	6:A:547:HOH:O	1.79	0.82
4:A:21:PRO:HG3	4:A:30:GLN:HG3	1.62	0.81
4:B:221:ASN:C	4:B:221:ASN:HD22	1.88	0.81
4:B:91:ARG:HH12	4:B:108:GLN:HE21	1.30	0.80
4:B:41:SER:HB2	4:B:46:CYS:H	1.46	0.79
1:D:14:DC:H2''	1:D:15:DG:C8	2.18	0.79
4:A:92:GLN:HG2	4:A:96:LYS:HE2	1.65	0.79
4:B:99:ARG:HD2	6:B:727:HOH:O	1.85	0.75
2:E:6:DC:H3'	3:G:7:DG:OP3	1.88	0.73
1:F:15:DG:H2''	1:F:16:DC:H5''	1.70	0.73
1:F:11:DG:C2'	1:F:12:DA:H5''	2.19	0.72
4:A:221:ASN:HD22	4:A:221:ASN:C	1.97	0.71
4:B:161:MET:CE	4:B:167:ARG:HH22	2.05	0.70
4:A:75:ARG:HH11	4:A:75:ARG:HG3	1.58	0.69
4:B:100:LYS:HD2	4:B:101:ASN:N	2.08	0.69
4:A:67:ARG:HD2	4:A:144:VAL:HG21	1.73	0.68
4:B:91:ARG:HH12	4:B:108:GLN:NE2	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:DC:H4'	4:A:131:SER:HA	1.74	0.68
1:F:12:DA:H2'	1:F:13:DT:C6	2.29	0.68
2:E:6:DC:H42	1:F:11:DG:H1	1.43	0.66
4:B:55:GLY:C	4:B:56:ILE:HD12	2.21	0.66
1:F:11:DG:H2''	1:F:12:DA:C5'	2.26	0.63
6:C:725:HOH:O	4:B:99:ARG:HD3	1.98	0.62
4:B:126:VAL:HG13	4:B:151:MET:HE2	1.81	0.62
6:A:472:HOH:O	4:B:20:PRO:HG2	2.00	0.60
4:B:91:ARG:HH22	4:B:108:GLN:NE2	1.99	0.60
4:A:75:ARG:HG3	4:A:75:ARG:NH1	2.16	0.59
1:F:15:DG:C2'	1:F:16:DC:H5''	2.31	0.59
4:B:161:MET:HE2	4:B:167:ARG:NH2	2.14	0.59
4:A:62:CYS:HA	4:A:148:ARG:NH2	2.17	0.58
3:G:7:DG:H2''	3:G:8:DC:H5'	1.85	0.58
4:B:220:HIS:O	4:B:222:PRO:HD3	2.03	0.58
4:A:41:SER:HB3	4:A:46:CYS:H	1.68	0.57
4:A:91:ARG:NH2	4:A:112:MET:HE1	2.20	0.57
4:A:198:LYS:CD	4:A:198:LYS:N	2.68	0.56
4:B:41:SER:HB2	4:B:46:CYS:N	2.19	0.56
4:A:194:GLN:O	4:A:198:LYS:HD3	2.05	0.56
1:D:15:DG:C2'	1:D:16:DC:H5''	2.28	0.55
2:E:6:DC:H5''	3:G:7:DG:P	2.47	0.55
4:A:137:GLN:HG3	4:A:161:MET:HE3	1.89	0.55
4:B:137:GLN:HG3	4:B:161:MET:HE3	1.88	0.55
4:B:192:LEU:HD11	4:B:196:TRP:CE2	2.43	0.54
4:B:84:ALA:HA	4:B:87:PHE:CZ	2.43	0.54
1:F:15:DG:H1'	1:F:16:DC:H5''	1.90	0.53
4:B:137:GLN:HG2	6:B:708:HOH:O	2.09	0.52
4:B:24:PHE:CZ	4:B:28:LYS:HD2	2.44	0.51
4:A:161:MET:CE	4:A:167:ARG:HH22	2.15	0.51
4:A:31:ALA:HB1	4:A:78:TRP:CZ3	2.47	0.51
4:B:126:VAL:CG1	4:B:151:MET:HE2	2.41	0.51
4:B:190:GLN:O	4:B:194:GLN:HG2	2.12	0.50
4:B:189:GLN:NE2	6:B:430:HOH:O	2.45	0.49
4:B:109:PHE:HA	4:B:112:MET:HE3	1.94	0.49
4:B:58:ASN:CG	4:B:61:THR:HG23	2.37	0.49
4:A:85:TRP:CG	4:A:132:ASN:HD22	2.30	0.49
4:B:211:ASP:O	4:B:215:LYS:HD3	2.13	0.49
4:A:61:THR:O	4:A:148:ARG:NH2	2.44	0.49
4:A:94:TRP:CH2	4:A:99:ARG:HB2	2.48	0.49
4:B:67:ARG:HD2	4:B:144:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:221:ASN:C	4:A:221:ASN:ND2	2.66	0.49
2:E:1:DG:H2''	2:E:2:DC:C5'	2.37	0.48
4:B:83:PRO:HD2	4:B:86:GLN:HG3	1.95	0.48
4:A:89:HIS:HA	4:A:94:TRP:CG	2.48	0.48
4:B:100:LYS:HB3	6:B:723:HOH:O	2.14	0.48
4:A:116:LEU:N	4:A:217:GLN:OE1	2.40	0.48
4:B:189:GLN:NE2	6:B:425:HOH:O	2.43	0.48
1:C:7:DG:H5''	4:B:127:ASN:ND2	2.30	0.47
4:A:25:SER:O	4:A:29:GLN:HG2	2.15	0.47
4:B:161:MET:CE	4:B:167:ARG:NH2	2.76	0.46
2:E:6:DC:N4	1:F:11:DG:H1	2.09	0.46
4:A:103:SER:O	4:A:110:ARG:HD2	2.14	0.46
4:A:67:ARG:CD	4:A:144:VAL:HG21	2.42	0.46
4:A:69:GLN:NE2	4:A:72:ARG:HG3	2.31	0.46
4:B:216:ILE:HD11	6:B:695:HOH:O	2.14	0.45
4:A:161:MET:HE2	4:A:167:ARG:NH2	2.19	0.45
4:B:57:PRO:HD3	4:B:76:ILE:HG12	1.98	0.45
1:F:11:DG:N7	6:F:716:HOH:O	2.36	0.45
4:B:78:TRP:CZ3	4:B:121:PRO:HD3	2.51	0.45
1:D:12:DA:C2'	1:D:13:DT:H72	2.47	0.45
3:G:7:DG:H2'	3:G:8:DC:C6	2.52	0.44
4:B:43:TYR:O	4:B:165:ARG:HD2	2.17	0.44
4:B:25:SER:HB3	6:B:621:HOH:O	2.17	0.44
1:F:15:DG:C1'	1:F:16:DC:H5''	2.47	0.44
4:B:172:ARG:NH2	4:B:200:TYR:O	2.42	0.44
4:B:39:PRO:HB2	4:B:48:ILE:O	2.18	0.43
4:B:83:PRO:HD2	4:B:86:GLN:CG	2.47	0.43
1:F:15:DG:H2''	1:F:16:DC:C5'	2.45	0.43
4:A:105:ASN:O	4:A:106:ASP:C	2.62	0.43
4:B:56:ILE:HD12	4:B:56:ILE:N	2.33	0.43
4:B:146:TYR:HB2	4:B:149:CYS:HB3	2.01	0.42
4:B:221:ASN:C	4:B:221:ASN:ND2	2.61	0.42
1:C:7:DG:O3'	4:B:77:GLU:HG2	2.19	0.42
4:A:176:TYR:HB2	4:A:221:ASN:ND2	2.34	0.42
4:B:99:ARG:NH2	4:B:113:GLU:OE2	2.53	0.42
4:B:220:HIS:CD2	6:B:412:HOH:O	2.73	0.42
4:A:190:GLN:OE1	4:A:194:GLN:NE2	2.52	0.42
4:A:157:GLN:NE2	6:A:643:HOH:O	2.25	0.42
4:A:93:CYS:O	4:A:101:ASN:HB3	2.19	0.42
1:F:12:DA:H2''	1:F:13:DT:H5'	2.02	0.41
4:A:108:GLN:OE1	4:A:112:MET:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:29:GLN:HG2	4:A:29:GLN:H	1.53	0.41
4:B:83:PRO:HD2	4:B:86:GLN:CD	2.46	0.41
4:A:19:ALA:N	4:A:20:PRO:HD3	2.35	0.41
4:B:89:HIS:HA	4:B:94:TRP:CG	2.55	0.41
4:B:204:GLU:CD	4:B:205:TRP:N	2.79	0.41
4:B:38:HIS:N	4:B:39:PRO:CD	2.83	0.41
4:B:91:ARG:HH22	4:B:108:GLN:HE22	1.69	0.41
4:B:175:LEU:HD12	4:B:175:LEU:HA	1.78	0.41
4:B:189:GLN:HG2	6:B:430:HOH:O	2.21	0.41
4:A:146:TYR:HB2	4:A:149:CYS:HB3	2.01	0.41
4:A:198:LYS:N	4:A:198:LYS:HD2	2.36	0.41
2:E:5:DT:H2"	2:E:6:DC:OP2	2.20	0.40
4:B:41:SER:O	4:B:45:GLY:HA2	2.22	0.40
4:B:179:GLN:NE2	6:B:433:HOH:O	2.54	0.40
4:A:105:ASN:ND2	6:A:686:HOH:O	2.55	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	
4	A	211/213 (99%)	201 (95%)	9 (4%)	1 (0%)	24	31
4	B	208/213 (98%)	195 (94%)	12 (6%)	1 (0%)	24	31
All	All	419/426 (98%)	396 (94%)	21 (5%)	2 (0%)	24	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	104	LYS
4	A	68	LYS

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	
4	A	185/185 (100%)	179 (97%)	6 (3%)	34	51
4	B	182/185 (98%)	165 (91%)	17 (9%)	8	11
All	All	367/370 (99%)	344 (94%)	23 (6%)	16	23

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	29	GLN
4	A	130	ARG
4	A	160	VAL
4	A	175	LEU
4	A	187	LYS
4	A	221	ASN
4	B	25	SER
4	B	54	LYS
4	B	92	GLN
4	B	95	GLN
4	B	100	LYS
4	B	108	GLN
4	B	119	LEU
4	B	130	ARG
4	B	139	ASN
4	B	151	MET
4	B	156	LYS
4	B	160	VAL
4	B	175	LEU
4	B	191	GLN
4	B	198	LYS
4	B	204	GLU
4	B	221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	36	GLN
4	A	51	GLN
4	A	65	GLN
4	A	69	GLN
4	A	105	ASN
4	A	134	ASN
4	A	190	GLN
4	A	191	GLN
4	A	194	GLN
4	A	221	ASN
4	A	225	GLN
4	A	226	GLN
4	A	229	GLN
4	B	51	GLN
4	B	69	GLN
4	B	70	GLN
4	B	86	GLN
4	B	92	GLN
4	B	108	GLN
4	B	134	ASN
4	B	179	GLN
4	B	188	GLN
4	B	189	GLN
4	B	194	GLN
4	B	221	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 2 ligands modelled in this entry, 2 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	8/8 (100%)	0.23	0 100 100	48, 51, 55, 58	0
1	D	8/8 (100%)	0.19	0 100 100	50, 54, 57, 64	0
1	F	8/8 (100%)	0.33	0 100 100	40, 52, 61, 62	0
2	E	6/6 (100%)	0.72	0 100 100	53, 56, 63, 64	0
3	G	2/2 (100%)	1.25	0 100 100	45, 45, 45, 49	0
4	A	213/213 (100%)	-0.47	0 100 100	10, 23, 44, 56	0
4	B	210/213 (98%)	-0.11	1 (0%) 87 87	14, 35, 54, 60	0
All	All	455/458 (99%)	-0.24	1 (0%) 91 91	10, 29, 55, 64	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	19	ALA	2.9

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	CA	A	300	1/1	0.98	0.02	24,24,24,24	0
5	CA	B	300	1/1	0.98	0.03	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.