



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 08:10 PM EDT

PDB ID : 1DGR  
Title : Refined crystal structure of canavalin from jack bean  
Authors : Ko, T.-P.; McPherson, A.  
Deposited on : 1999-11-25  
Resolution : 2.60 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.

The types of validation reports are described at

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

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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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.36.2  
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) : 2.36.2

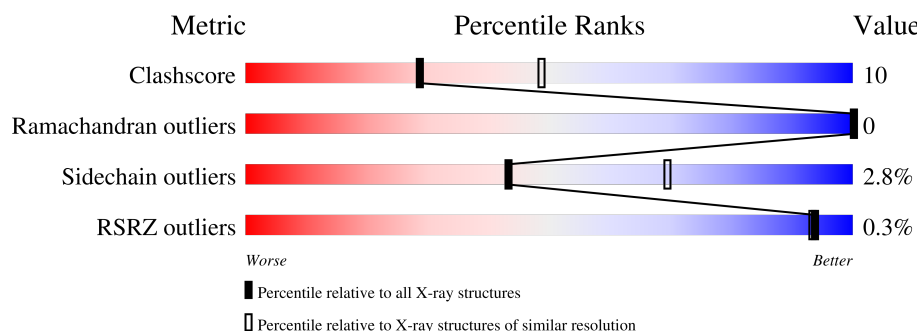
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	A	178	 81% 18% •
1	B	178	 77% 22% •
1	C	178	 81% 17% •
2	N	79	 78% 16% • •
2	V	79	 75% 20% • •
2	X	79	 77% 16% • 5%

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Mol	Chain	Length	Quality of chain
3	M	93	<div><div>%</div><div><div></div></div><div>67%31%<div>••</div></div></div>
3	W	93	<div><div></div><div>75%23%<div>•</div></div></div>
3	Y	93	<div><div></div><div>72%27%<div>•</div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8530 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 protein called CANAVALIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1457	932	246	277	2			
1	B	178	Total	C	N	O	S	0	0	0
			1457	932	246	277	2			
1	C	178	Total	C	N	O	S	0	0	0
			1457	932	246	277	2			

- Molecule 2 is a protein called CANAVALIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	75	Total	C	N	O	S	0	0	0
			601	379	105	115	2			
2	V	76	Total	C	N	O	S	0	0	0
			610	384	106	118	2			
2	N	76	Total	C	N	O	S	0	0	0
			610	384	106	118	2			

- Molecule 3 is a protein called CANAVALIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	93	Total	C	N	O	S	0	0	0
			721	450	125	144	2			
3	W	93	Total	C	N	O	S	0	0	0
			721	450	125	144	2			
3	M	92	Total	C	N	O	S	0	0	0
			713	445	124	143	1			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total	O	P	0	0
			5	4	1		
4	V	1	Total	O	P	0	0
			5	4	1		
4	N	1	Total	O	P	0	0
			5	4	1		

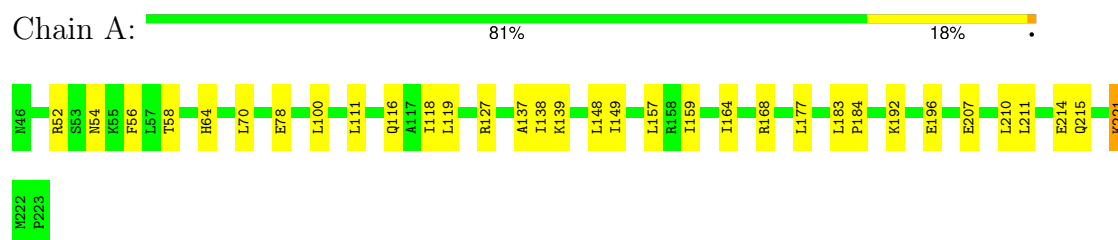
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	X	18	Total	O	0	0
			18	18		
5	Y	17	Total	O	0	0
			17	17		
5	B	23	Total	O	0	0
			23	23		
5	V	8	Total	O	0	0
			8	8		
5	W	15	Total	O	0	0
			15	15		
5	C	30	Total	O	0	0
			30	30		
5	N	17	Total	O	0	0
			17	17		
5	M	13	Total	O	0	0
			13	13		

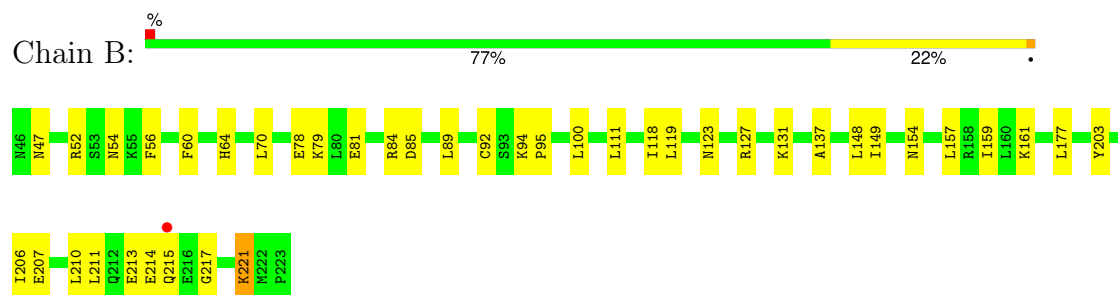
### 3 Residue-property plots

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.

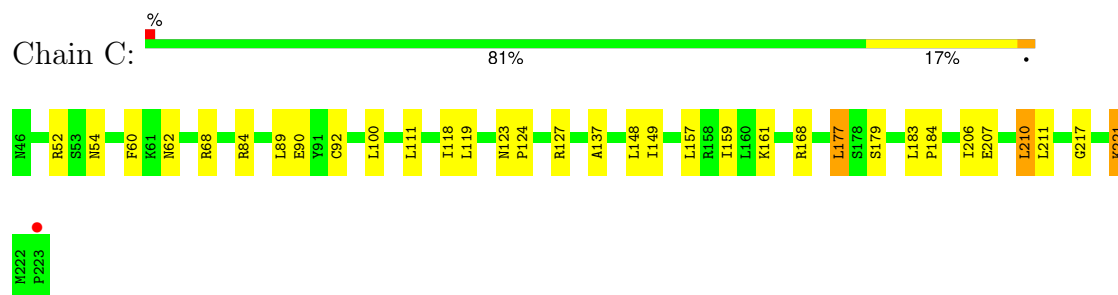
#### • Molecule 1: CANAVALIN



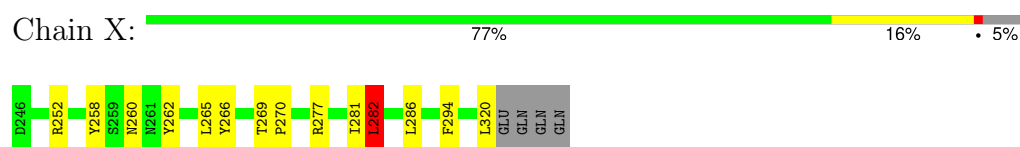
#### • Molecule 1: CANAVALIN



#### • Molecule 1: CANAVALIN

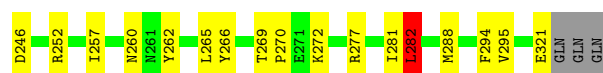


#### • Molecule 2: CANAVALIN




#### • Molecule 2: CANAVALIN

Chain V:  75% 20% . .



• Molecule 2: CANAVALIN

Chain N:  78% 16% . .




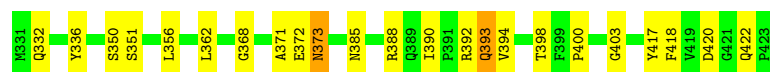
• Molecule 3: CANAVALIN

Chain Y:  72% 27% .



• Molecule 3: CANAVALIN

Chain W:  75% 23% .



• Molecule 3: CANAVALIN

Chain M:  67% 31% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.50Å 150.30Å 133.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 2.60 32.31 – 2.57	Depositor EDS
% Data completeness (in resolution range)	67.8 (200.00-2.60) 66.0 (32.31-2.57)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.57Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.180 , 0.226 0.181 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: PO4

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	0.40	0/1488	0.61	0/2016
1	B	0.41	0/1488	0.63	0/2016
1	C	0.43	0/1488	0.64	0/2016
2	N	0.43	0/620	0.73	1/840 (0.1%)
2	V	0.40	0/620	0.72	1/840 (0.1%)
2	X	0.46	0/611	0.72	1/828 (0.1%)
3	M	0.38	0/724	0.63	0/980
3	W	0.37	0/732	0.64	0/990
3	Y	0.43	0/732	0.66	0/990
All	All	0.41	0/8503	0.65	3/11516 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	282	LEU	CA-CB-CG	5.88	128.82	115.30
2	X	282	LEU	CA-CB-CG	5.81	128.67	115.30
2	N	282	LEU	CA-CB-CG	5.28	127.45	115.30

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	1457	0	1447	23	0
1	B	1457	0	1447	36	0
1	C	1457	0	1447	24	0
2	N	610	0	604	14	0
2	V	610	0	604	19	0
2	X	601	0	598	16	0
3	M	713	0	697	21	0
3	W	721	0	706	20	0
3	Y	721	0	706	19	0
4	N	5	0	0	0	0
4	V	5	0	0	0	0
4	X	5	0	0	0	0
5	A	27	0	0	0	0
5	B	23	0	0	5	0
5	C	30	0	0	1	0
5	M	13	0	0	0	0
5	N	17	0	0	0	0
5	V	8	0	0	1	0
5	W	15	0	0	0	0
5	X	18	0	0	0	0
5	Y	17	0	0	0	0
All	All	8530	0	8256	161	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 10.

All (161) 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:W:394:VAL:O	3:W:398:THR:HG23	1.72	0.90
3:Y:394:VAL:O	3:Y:398:THR:HG23	1.77	0.83
1:B:221:LYS:HD3	1:B:221:LYS:H	1.44	0.82
1:C:161:LYS:NZ	5:C:631:HOH:O	2.18	0.76
3:M:394:VAL:O	3:M:398:THR:HG23	1.88	0.73
3:Y:391:PRO:HG3	1:C:127:ARG:CZ	2.19	0.73
1:A:100:LEU:HD22	3:W:398:THR:HG22	1.70	0.71
3:W:420:ASP:OD1	3:W:422:GLN:HG2	1.94	0.68
2:V:260:ASN:HB3	2:V:262:TYR:H	1.59	0.67
1:B:213:GLU:OE1	5:B:546:HOH:O	2.13	0.66
3:W:385:ASN:HB3	3:W:388:ARG:HD3	1.79	0.64
1:B:221:LYS:HD3	1:B:221:LYS:N	2.12	0.63
2:N:295:VAL:HG22	3:M:417:TYR:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:LYS:HD3	1:C:221:LYS:H	1.64	0.62
2:N:260:ASN:HB3	2:N:262:TYR:H	1.64	0.62
2:X:260:ASN:HB3	2:X:262:TYR:H	1.64	0.61
3:Y:420:ASP:OD1	3:Y:422:GLN:HG2	1.99	0.61
1:B:148:LEU:HD21	1:B:159:ILE:CD1	2.31	0.61
1:A:221:LYS:HD3	1:A:221:LYS:H	1.66	0.61
3:M:420:ASP:OD1	3:M:422:GLN:HG2	2.01	0.60
2:V:295:VAL:HG22	3:W:417:TYR:O	2.01	0.60
1:B:207:GLU:HA	1:B:211:LEU:HB2	1.84	0.60
1:A:210:LEU:HA	3:W:400:PRO:HD2	1.84	0.59
1:B:52:ARG:HB2	1:B:54:ASN:OD1	2.03	0.59
1:B:100:LEU:HD22	3:M:398:THR:HG22	1.84	0.58
1:A:168:ARG:HH21	1:B:78:GLU:HG2	1.67	0.58
1:B:148:LEU:HD21	1:B:159:ILE:HD12	1.84	0.57
1:A:119:LEU:HD13	1:A:148:LEU:HD13	1.85	0.57
1:C:68:ARG:NH1	1:C:90:GLU:OE1	2.36	0.57
3:Y:390:ILE:HG22	3:Y:394:VAL:HG13	1.87	0.57
1:B:214:GLU:HG3	1:B:215:GLN:N	2.21	0.56
2:X:282:LEU:HD22	3:Y:368:GLY:HA3	1.87	0.56
1:B:154:ASN:HA	5:B:643:HOH:O	2.05	0.56
1:A:118:ILE:HB	1:A:149:ILE:HB	1.88	0.55
1:B:210:LEU:HA	3:M:400:PRO:HD2	1.88	0.55
2:X:282:LEU:C	2:X:282:LEU:HD23	2.28	0.55
2:N:265:LEU:HD13	2:N:286:LEU:HD13	1.88	0.54
3:Y:392:ARG:HH21	3:Y:407:GLU:CD	2.10	0.54
3:W:390:ILE:HG22	3:W:394:VAL:HG13	1.90	0.54
2:N:282:LEU:C	2:N:282:LEU:HD23	2.27	0.54
1:A:127:ARG:HH11	1:A:127:ARG:HG2	1.73	0.54
1:A:78:GLU:HG2	1:C:168:ARG:HH21	1.73	0.54
3:Y:400:PRO:HD2	1:C:210:LEU:HA	1.90	0.53
3:W:392:ARG:HG2	3:W:403:GLY:HA3	1.91	0.53
1:A:127:ARG:HG2	1:A:127:ARG:NH1	2.23	0.53
2:N:282:LEU:HD22	3:M:368:GLY:HA3	1.91	0.53
1:B:79:LYS:HE3	2:V:321:GLU:OE1	2.09	0.52
1:C:118:ILE:HB	1:C:149:ILE:HB	1.90	0.52
3:Y:350:SER:O	3:Y:351:SER:HB2	2.09	0.52
2:X:258:TYR:CE2	2:X:265:LEU:HD23	2.44	0.52
2:V:282:LEU:HD22	3:W:368:GLY:HA3	1.91	0.52
1:B:47:ASN:ND2	3:W:336:TYR:HB3	2.25	0.51
1:B:92:CYS:SG	5:B:649:HOH:O	2.58	0.51
1:A:64:HIS:NE2	1:A:221:LYS:HD2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:NH1	5:B:660:HOH:O	2.43	0.51
2:X:270:PRO:O	2:X:277:ARG:HB3	2.09	0.51
2:V:260:ASN:HD22	3:W:418:PHE:HB2	1.76	0.51
2:V:246:ASP:HA	5:V:635:HOH:O	2.11	0.51
1:C:111:LEU:HD13	1:C:137:ALA:HB2	1.93	0.50
2:N:282:LEU:HD23	2:N:282:LEU:O	2.10	0.50
3:M:354:VAL:HG22	3:M:355:ALA:N	2.27	0.50
2:V:277:ARG:HH11	2:V:277:ARG:HG3	1.76	0.50
3:M:385:ASN:HB3	3:M:388:ARG:HD3	1.94	0.50
1:A:183:LEU:HG	1:A:184:PRO:HD2	1.93	0.50
2:V:270:PRO:O	2:V:277:ARG:HB3	2.10	0.50
2:X:258:TYR:CD2	2:X:265:LEU:HD23	2.47	0.50
2:X:282:LEU:HD23	2:X:282:LEU:O	2.12	0.50
3:Y:389:GLN:HG3	1:C:123:ASN:O	2.11	0.50
1:B:119:LEU:HD13	1:B:148:LEU:HD13	1.94	0.49
2:X:281:ILE:HG22	2:X:282:LEU:N	2.27	0.49
2:X:320:LEU:HD23	3:Y:333:LEU:HA	1.95	0.49
1:B:127:ARG:CZ	3:M:391:PRO:HG3	2.43	0.49
1:A:52:ARG:HB2	1:A:54:ASN:OD1	2.13	0.49
3:W:350:SER:O	3:W:351:SER:HB2	2.12	0.49
1:C:60:PHE:CE1	1:C:62:ASN:HB2	2.47	0.48
3:M:378:PHE:HB2	3:M:384:GLU:O	2.13	0.48
1:B:111:LEU:HD13	1:B:137:ALA:HB2	1.96	0.48
1:B:56:PHE:CE1	1:B:70:LEU:HD13	2.48	0.48
1:C:206:ILE:HG23	1:C:210:LEU:HD11	1.94	0.48
2:N:270:PRO:O	2:N:277:ARG:HB3	2.13	0.48
2:V:281:ILE:HG22	2:V:282:LEU:N	2.27	0.48
1:A:207:GLU:HA	1:A:211:LEU:HB2	1.95	0.48
2:N:269:THR:HB	2:N:270:PRO:HD2	1.96	0.48
2:V:257:ILE:HD11	2:V:265:LEU:HD23	1.94	0.48
1:C:207:GLU:HA	1:C:211:LEU:HB2	1.96	0.48
2:N:282:LEU:HB3	3:M:371:ALA:CB	2.44	0.48
1:B:89:LEU:HB2	1:B:161:LYS:HB2	1.96	0.48
3:Y:356:LEU:HD23	3:Y:356:LEU:N	2.29	0.47
3:Y:398:THR:HG22	1:C:100:LEU:HD22	1.95	0.47
2:X:281:ILE:CD1	3:Y:369:VAL:HG12	2.45	0.47
3:M:390:ILE:HG22	3:M:394:VAL:HG13	1.96	0.47
3:Y:354:VAL:HG22	3:Y:355:ALA:N	2.30	0.47
1:A:78:GLU:H	1:A:78:GLU:CD	2.18	0.47
3:Y:392:ARG:HG3	3:Y:403:GLY:HA3	1.97	0.47
2:V:277:ARG:HG3	2:V:277:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PHE:HZ	1:B:217:GLY:HA3	1.80	0.47
2:N:254:ARG:HG2	2:N:254:ARG:HH11	1.80	0.47
3:M:350:SER:O	3:M:351:SER:HB2	2.14	0.46
1:B:214:GLU:HB2	3:M:400:PRO:HA	1.98	0.46
2:X:252:ARG:HG2	2:X:266:TYR:CD2	2.51	0.46
1:A:56:PHE:CE1	1:A:70:LEU:HD13	2.50	0.46
1:A:116:GLN:O	1:A:157:LEU:HD13	2.15	0.46
1:C:52:ARG:HB2	1:C:54:ASN:OD1	2.16	0.46
1:B:118:ILE:HB	1:B:149:ILE:HB	1.98	0.46
2:V:282:LEU:C	2:V:282:LEU:HD23	2.36	0.45
2:N:281:ILE:HG22	2:N:282:LEU:N	2.30	0.45
1:B:203:TYR:O	1:B:206:ILE:N	2.49	0.45
1:B:221:LYS:N	1:B:221:LYS:CD	2.80	0.45
1:C:89:LEU:HB2	1:C:161:LYS:HB2	1.99	0.45
1:B:127:ARG:HH11	1:B:127:ARG:HG2	1.82	0.44
1:B:85:ASP:OD2	5:B:642:HOH:O	2.21	0.44
2:V:282:LEU:HB3	3:W:371:ALA:CB	2.48	0.44
1:B:127:ARG:HG2	1:B:127:ARG:NH1	2.33	0.44
1:A:111:LEU:HD13	1:A:137:ALA:HB2	2.00	0.43
2:V:252:ARG:HG2	2:V:266:TYR:CD2	2.53	0.43
1:C:118:ILE:O	1:C:148:LEU:HD12	2.18	0.43
1:B:123:ASN:O	3:M:389:GLN:HG3	2.19	0.43
3:W:372:GLU:O	3:W:373:ASN:HB2	2.16	0.43
2:V:282:LEU:HD23	2:V:282:LEU:O	2.18	0.43
1:C:119:LEU:HD13	1:C:148:LEU:HD13	2.01	0.43
1:C:183:LEU:HG	1:C:184:PRO:HD2	1.99	0.43
2:X:269:THR:HB	2:X:270:PRO:HD2	2.00	0.43
2:N:288:MET:HE3	3:M:362:LEU:HD23	2.01	0.43
3:W:385:ASN:CB	3:W:388:ARG:HD3	2.49	0.43
1:B:131:LYS:HE3	1:B:131:LYS:HB2	1.81	0.43
3:W:372:GLU:O	3:W:373:ASN:CB	2.66	0.43
1:A:138:ILE:HG12	1:A:139:LYS:N	2.34	0.42
3:M:334:ARG:HD2	3:M:335:ARG:H	1.84	0.42
2:X:286:LEU:O	3:Y:363:ASN:HA	2.19	0.42
3:Y:334:ARG:HD2	3:Y:335:ARG:H	1.84	0.42
2:V:288:MET:CE	3:W:362:LEU:HD23	2.49	0.42
1:A:221:LYS:HD3	1:A:221:LYS:N	2.32	0.42
1:B:119:LEU:CD1	1:B:148:LEU:HD13	2.50	0.42
2:V:252:ARG:HH11	2:V:252:ARG:HG3	1.84	0.42
1:B:94:LYS:HB3	1:B:95:PRO:CD	2.49	0.42
2:N:269:THR:OG1	2:N:272:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HE3	1:A:196:GLU:OE1	2.19	0.42
2:X:260:ASN:ND2	3:Y:418:PHE:O	2.52	0.42
1:C:221:LYS:HD3	1:C:221:LYS:N	2.32	0.42
3:M:402:SER:O	3:M:406:VAL:HG23	2.20	0.41
3:M:422:GLN:HA	3:M:423:PRO:HD3	1.85	0.41
2:X:281:ILE:CG2	2:X:282:LEU:N	2.84	0.41
1:A:148:LEU:HD21	1:A:159:ILE:CD1	2.50	0.41
2:V:282:LEU:HB3	3:W:371:ALA:HB2	2.02	0.41
1:C:92:CYS:HA	1:C:157:LEU:O	2.20	0.41
1:A:214:GLU:HG3	1:A:215:GLN:N	2.36	0.41
1:B:92:CYS:HA	1:B:157:LEU:O	2.20	0.41
1:B:94:LYS:HB3	1:B:95:PRO:HD2	2.02	0.41
1:C:60:PHE:CZ	1:C:217:GLY:HA3	2.56	0.41
1:C:148:LEU:HD21	1:C:159:ILE:CD1	2.51	0.41
1:A:164:ILE:N	1:A:164:ILE:HD12	2.36	0.40
3:M:356:LEU:N	3:M:356:LEU:HD23	2.36	0.40
2:X:282:LEU:HB3	3:Y:371:ALA:CB	2.52	0.40
3:M:392:ARG:NH1	3:M:404:GLU:HG3	2.35	0.40
1:B:64:HIS:NE2	1:B:221:LYS:HD2	2.36	0.40
3:W:356:LEU:N	3:W:356:LEU:HD23	2.36	0.40
2:N:254:ARG:HG2	2:N:254:ARG:NH1	2.37	0.40
2:V:269:THR:OG1	2:V:272:LYS:HE2	2.21	0.40
3:W:393:GLN:H	3:W:393:GLN:CD	2.21	0.40
1:C:123:ASN:HB3	1:C:124:PRO:HD2	2.03	0.40
1:C:177:LEU:HD12	1:C:177:LEU:HA	1.92	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	176/178 (99%)	163 (93%)	13 (7%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	176/178 (99%)	163 (93%)	13 (7%)	0	100	100
1	C	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
2	N	74/79 (94%)	72 (97%)	2 (3%)	0	100	100
2	V	74/79 (94%)	72 (97%)	2 (3%)	0	100	100
2	X	73/79 (92%)	71 (97%)	2 (3%)	0	100	100
3	M	90/93 (97%)	87 (97%)	3 (3%)	0	100	100
3	W	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
3	Y	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
All	All	1021/1050 (97%)	975 (96%)	46 (4%)	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	165/165 (100%)	162 (98%)	3 (2%)	59	80
1	B	165/165 (100%)	162 (98%)	3 (2%)	59	80
1	C	165/165 (100%)	160 (97%)	5 (3%)	41	67
2	N	68/71 (96%)	66 (97%)	2 (3%)	42	68
2	V	68/71 (96%)	66 (97%)	2 (3%)	42	68
2	X	67/71 (94%)	65 (97%)	2 (3%)	41	67
3	M	78/79 (99%)	75 (96%)	3 (4%)	33	59
3	W	79/79 (100%)	76 (96%)	3 (4%)	33	59
3	Y	79/79 (100%)	76 (96%)	3 (4%)	33	59
All	All	934/945 (99%)	908 (97%)	26 (3%)	43	69

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	177	LEU
1	A	221	LYS
2	X	282	LEU
2	X	294	PHE
3	Y	356	LEU
3	Y	373	ASN
3	Y	393	GLN
1	B	81	GLU
1	B	177	LEU
1	B	221	LYS
2	V	282	LEU
2	V	294	PHE
3	W	332	GLN
3	W	373	ASN
3	W	393	GLN
1	C	84	ARG
1	C	177	LEU
1	C	179	SER
1	C	210	LEU
1	C	221	LYS
2	N	282	LEU
2	N	294	PHE
3	M	356	LEU
3	M	373	ASN
3	M	393	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	155	GLN
1	A	212	GLN
2	X	261	ASN
2	X	287	GLN
1	B	63	GLN
1	B	71	GLN
1	B	155	GLN
1	B	212	GLN
2	V	261	ASN
3	W	422	GLN
1	C	63	GLN
1	C	155	GLN

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Mol	Chain	Res	Type
1	C	212	GLN
2	N	261	ASN
2	N	287	GLN
3	M	412	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](#)

3 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	$\# Z  > 2$
4	PO4	V	2500	-	4,4,4	1.59	0	6,6,6	0.44	0
4	PO4	N	3500	-	4,4,4	1.59	0	6,6,6	0.46	0
4	PO4	X	1500	-	4,4,4	1.57	0	6,6,6	0.45	0

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

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, 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	A	178/178 (100%)	-0.56	0 100 100	18, 35, 56, 61	0
1	B	178/178 (100%)	-0.47	1 (0%) 89 88	22, 37, 58, 61	0
1	C	178/178 (100%)	-0.59	1 (0%) 89 88	17, 30, 47, 55	0
2	N	76/79 (96%)	-0.58	0 100 100	17, 33, 44, 48	0
2	V	76/79 (96%)	-0.63	0 100 100	18, 38, 44, 48	0
2	X	75/79 (94%)	-0.74	0 100 100	11, 26, 33, 40	0
3	M	92/93 (98%)	-0.46	1 (1%) 80 78	19, 38, 52, 54	0
3	W	93/93 (100%)	-0.47	0 100 100	24, 40, 53, 57	0
3	Y	93/93 (100%)	-0.60	0 100 100	18, 29, 43, 53	0
All	All	1039/1050 (98%)	-0.56	3 (0%) 94 93	11, 33, 52, 61	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	GLN	3.2
3	M	422	GLN	2.3
1	C	223	PRO	2.3

### 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( $\text{\AA}^2$ )	Q<0.9
4	PO4	V	2500	5/5	0.96	0.26	63,63,64,64	0
4	PO4	X	1500	5/5	0.97	0.15	66,66,66,66	0
4	PO4	N	3500	5/5	0.97	0.23	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.