



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WUV
Title : Crystal structure of native Canavalia gladiata lectin (CGL): a tetrameric ConA-like lectin
Authors : Freitas, B.T.; Delatorre, P.; Moreno, F.B.M.B.; Rocha, B.A.M.; Souza, E.P.; Canduri, F.; Cardoso, A.L.H.; Sampaio, A.H.; Azevedo Jr., W.F.; Cavada, B.S.
Deposited on : 2004-12-09
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

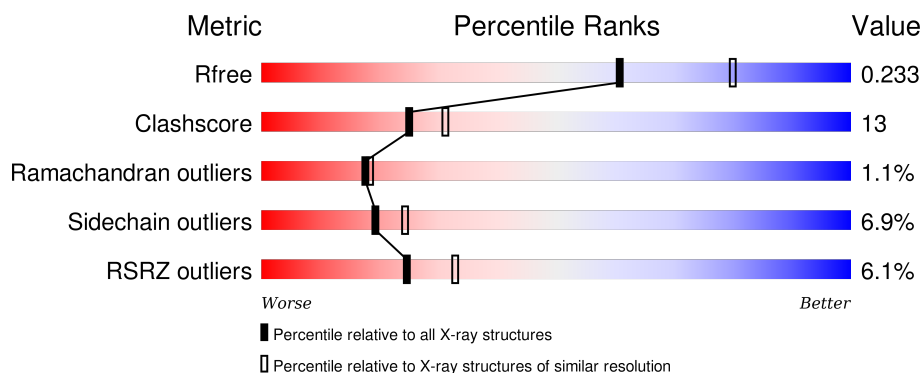
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>••</div> </div> </div>
1	D	237	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>••</div> </div> </div>
1	G	237	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>5%</div> </div> </div>
1	J	237	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>5%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7640 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 Concanavalin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1805	1138	303	362	2			
1	D	237	Total	C	N	O	S	0	0	0
			1805	1138	303	362	2			
1	G	237	Total	C	N	O	S	0	0	0
			1805	1138	303	362	2			
1	J	237	Total	C	N	O	S	0	0	0
			1805	1138	303	362	2			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	J	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Ca	0	0
			1	1		
3	J	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

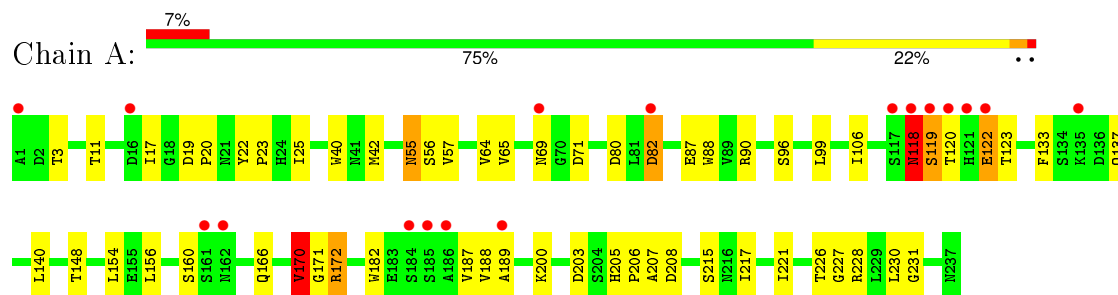
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total 114	O 114	0	0
4	D	101	Total 101	O 101	0	0
4	G	99	Total 99	O 99	0	0
4	J	98	Total 98	O 98	0	0

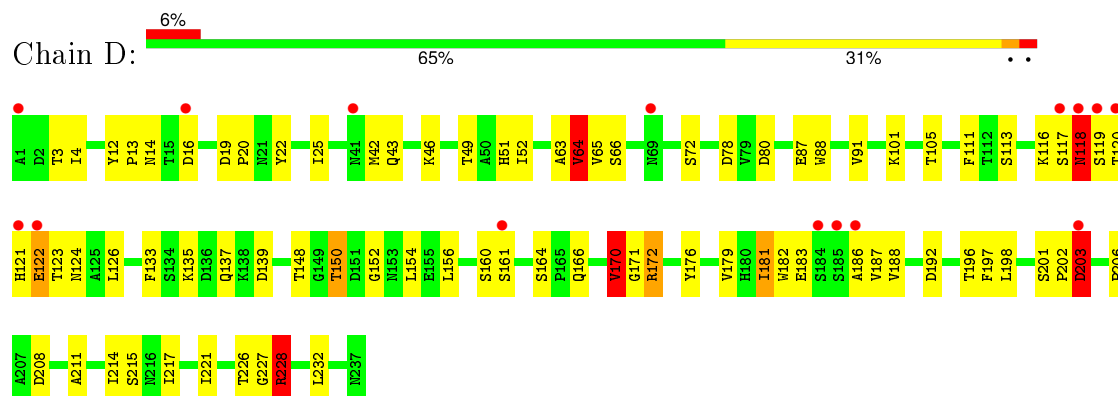
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

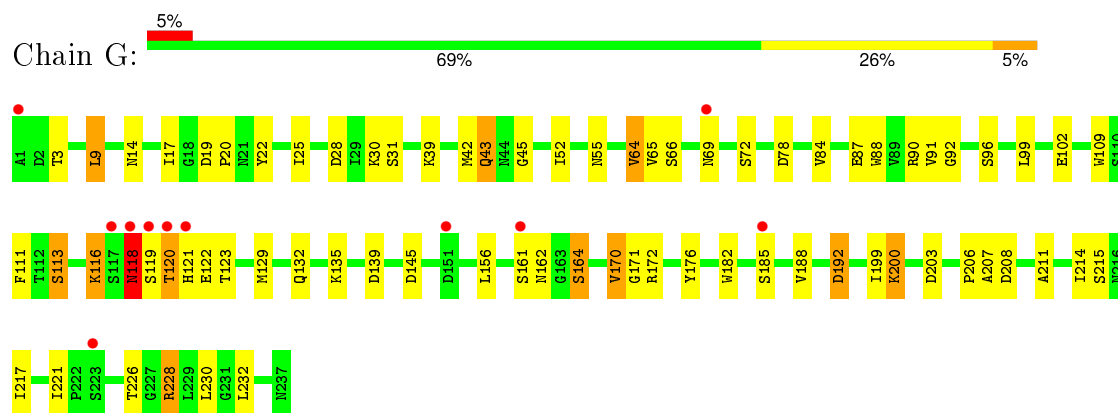
• Molecule 1: Concanavalin A



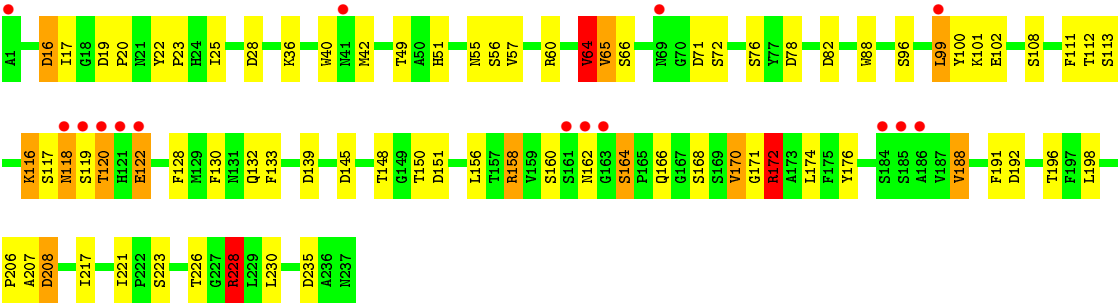
• Molecule 1: Concanavalin A



• Molecule 1: Concanavalin A



• Molecule 1: Concanavalin A



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.90Å 115.35Å 241.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (10.00-2.30) 97.9 (10.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.184 , 0.233 0.187 , 0.233	Depositor DCC
R_{free} test set	3062 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 61881 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7640	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MN

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	0.99	0/1847	1.06	8/2516 (0.3%)
1	D	0.99	1/1847 (0.1%)	1.18	13/2516 (0.5%)
1	G	0.96	1/1847 (0.1%)	1.05	6/2516 (0.2%)
1	J	0.95	1/1847 (0.1%)	1.11	16/2516 (0.6%)
All	All	0.97	3/7388 (0.0%)	1.10	43/10064 (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	D	0	2
1	G	0	1
1	J	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	16	ASP	CB-CG	8.58	1.69	1.51
1	G	43	GLN	CG-CD	6.53	1.66	1.51
1	J	65	VAL	CB-CG2	-5.97	1.40	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	ASP	CB-CG-OD2	12.34	129.40	118.30
1	D	228	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	D	228	ARG	NE-CZ-NH1	11.08	125.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	G	78	ASP	CB-CG-OD2	8.81	126.23	118.30
1	J	228	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	J	64	VAL	CB-CA-C	-7.71	96.75	111.40
1	D	64	VAL	CB-CA-C	-7.59	96.98	111.40
1	G	64	VAL	CB-CA-C	-7.39	97.36	111.40
1	J	172	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	G	192	ASP	CB-CG-OD2	7.05	124.64	118.30
1	D	80	ASP	CB-CG-OD2	7.04	124.63	118.30
1	A	82	ASP	CB-CG-OD1	6.84	124.45	118.30
1	A	64	VAL	CB-CA-C	-6.77	98.54	111.40
1	D	170	VAL	CG1-CB-CG2	6.61	121.48	110.90
1	J	228	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	G	139	ASP	CB-CG-OD2	6.57	124.21	118.30
1	J	71	ASP	CB-CG-OD2	6.57	124.21	118.30
1	J	78	ASP	CB-CG-OD2	6.54	124.19	118.30
1	J	28	ASP	CB-CG-OD2	6.40	124.06	118.30
1	J	192	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	170	VAL	CB-CA-C	-6.22	99.58	111.40
1	J	16	ASP	CB-CG-OD2	6.12	123.81	118.30
1	G	203	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	170	VAL	CG1-CB-CG2	5.92	120.38	110.90
1	D	78	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	203	ASP	CB-CG-OD2	5.87	123.58	118.30
1	J	19	ASP	CB-CG-OD2	5.77	123.49	118.30
1	J	208	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	170	VAL	CB-CA-C	-5.61	100.74	111.40
1	A	170	VAL	CA-CB-CG2	5.55	119.23	110.90
1	J	99	LEU	CB-CG-CD2	5.48	120.32	111.00
1	D	16	ASP	OD1-CG-OD2	-5.42	113.00	123.30
1	J	235	ASP	CB-CG-OD2	5.40	123.16	118.30
1	G	145	ASP	CB-CG-OD2	5.38	123.14	118.30
1	J	99	LEU	CB-CG-CD1	5.35	120.09	111.00
1	A	172	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	J	16	ASP	N-CA-CB	-5.20	101.24	110.60
1	D	154	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	19	ASP	CB-CG-OD2	5.17	122.96	118.30
1	J	145	ASP	CB-CG-OD2	5.13	122.91	118.30
1	D	172	ARG	CB-CG-CD	-5.01	98.57	111.60
1	D	203	ASP	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	118	ASN	Peptide
1	D	123	THR	Peptide
1	G	118	ASN	Peptide
1	J	118	ASN	Peptide

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	1805	0	1751	35	0
1	D	1805	0	1751	51	0
1	G	1805	0	1751	52	0
1	J	1805	0	1751	45	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
4	A	114	0	0	0	0
4	D	101	0	0	1	0
4	G	99	0	0	1	0
4	J	98	0	0	1	0
All	All	7640	0	7004	181	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 13.

All (181) 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)
1:G:43:GLN:NE2	1:G:69:ASN:HD21	1.16	1.41
1:G:43:GLN:HE22	1:G:69:ASN:ND2	1.24	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:SER:O	1:J:122:GLU:HG2	1.51	1.07
1:G:25:ILE:HD12	1:G:65:VAL:HG23	1.46	0.97
1:G:42:MET:HE2	1:G:206:PRO:HG2	1.46	0.96
1:D:160:SER:HB3	1:D:166:GLN:NE2	1.81	0.95
1:D:25:ILE:HD12	1:D:65:VAL:HG23	1.49	0.92
1:J:170:VAL:HG22	1:J:226:THR:HG22	1.55	0.88
1:J:25:ILE:HD12	1:J:65:VAL:HG23	1.56	0.87
1:J:160:SER:HB3	1:J:166:GLN:NE2	1.89	0.86
1:G:43:GLN:NE2	1:G:69:ASN:ND2	1.97	0.85
1:A:25:ILE:HD12	1:A:65:VAL:HG23	1.58	0.84
1:A:119:SER:HB2	1:A:122:GLU:HG3	1.60	0.83
1:G:25:ILE:HD12	1:G:65:VAL:CG2	2.09	0.83
1:D:160:SER:HB3	1:D:166:GLN:HE22	1.41	0.82
1:J:119:SER:HB2	1:J:122:GLU:HG3	1.62	0.80
1:G:42:MET:CE	1:G:206:PRO:HG2	2.10	0.80
1:A:25:ILE:HD12	1:A:65:VAL:CG2	2.13	0.79
1:D:25:ILE:HD12	1:D:65:VAL:CG2	2.12	0.79
1:A:170:VAL:HG22	1:A:226:THR:HG22	1.63	0.79
1:J:119:SER:C	1:J:122:GLU:HG2	2.02	0.79
1:J:88:TRP:HB3	1:J:217:ILE:HD11	1.66	0.78
1:G:119:SER:HB2	1:G:122:GLU:HG3	1.66	0.76
1:D:156:LEU:O	1:D:171:GLY:HA3	1.87	0.75
1:G:66:SER:HB3	1:G:72:SER:CB	2.17	0.75
1:G:172:ARG:HD2	1:G:221:ILE:HG12	1.69	0.74
1:D:202:PRO:C	1:D:203:ASP:O	2.24	0.70
1:J:16:ASP:OD2	1:J:228:ARG:NH2	2.24	0.70
1:A:87:GLU:HG2	1:A:182:TRP:O	1.91	0.69
1:D:66:SER:HB3	1:D:72:SER:CB	2.22	0.69
1:D:170:VAL:HG22	1:D:226:THR:HG22	1.74	0.68
1:D:88:TRP:HB3	1:D:217:ILE:HD11	1.77	0.67
1:G:116:LYS:HD3	1:G:123:THR:OG1	1.94	0.67
1:G:162:ASN:OD1	1:G:164:SER:HB2	1.95	0.67
1:G:42:MET:HE2	1:G:206:PRO:CG	2.22	0.67
1:A:137:GLN:HG2	1:A:140:LEU:HD12	1.76	0.66
1:J:66:SER:HB3	1:J:72:SER:HB2	1.76	0.66
1:D:87:GLU:HG3	1:D:182:TRP:O	1.96	0.66
1:D:66:SER:HB3	1:D:72:SER:HB3	1.77	0.66
1:G:66:SER:HB3	1:G:72:SER:HB2	1.78	0.66
1:G:118:ASN:H	1:G:118:ASN:ND2	1.94	0.65
1:J:42:MET:HE1	1:J:206:PRO:HG3	1.77	0.65
1:D:228:ARG:HD2	4:D:268:HOH:O	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:160:SER:HB3	1:J:166:GLN:HE21	1.60	0.64
1:G:118:ASN:H	1:G:118:ASN:HD22	1.43	0.64
1:G:116:LYS:HG3	1:G:188:VAL:HB	1.80	0.64
1:A:80:ASP:OD1	1:A:82:ASP:HB2	2.00	0.62
1:D:170:VAL:HG22	1:D:226:THR:CG2	2.30	0.62
1:J:42:MET:CE	1:J:206:PRO:HG3	2.30	0.62
1:J:17:ILE:HD13	1:J:228:ARG:HD3	1.83	0.61
1:G:66:SER:HB3	1:G:72:SER:HB3	1.84	0.59
1:J:66:SER:HB3	1:J:72:SER:CB	2.32	0.59
1:A:160:SER:HB3	1:A:166:GLN:NE2	2.18	0.59
1:J:158:ARG:HH11	1:J:158:ARG:HG3	1.68	0.59
1:J:60:ARG:HD3	1:J:76:SER:HB3	1.85	0.59
1:D:118:ASN:H	1:D:118:ASN:ND2	2.00	0.58
1:J:172:ARG:HD2	1:J:221:ILE:HG12	1.84	0.58
1:G:120:THR:HG22	1:G:121:HIS:HD2	1.67	0.58
1:A:170:VAL:HG22	1:A:226:THR:CG2	2.33	0.57
1:D:137:GLN:NE2	1:D:139:ASP:OD1	2.28	0.57
1:G:42:MET:CE	1:G:206:PRO:CG	2.83	0.56
1:G:119:SER:O	1:G:122:GLU:HG2	2.05	0.56
1:D:133:PHE:O	1:D:152:GLY:HA2	2.06	0.56
1:D:25:ILE:CD1	1:D:65:VAL:HG23	2.29	0.56
1:G:30:LYS:HD2	1:G:84:VAL:HG13	1.88	0.56
1:D:66:SER:HB3	1:D:72:SER:HB2	1.88	0.55
1:G:43:GLN:HE22	1:G:69:ASN:HD21	0.56	0.54
1:A:20:PRO:HB2	1:A:22:TYR:CZ	2.42	0.54
1:A:90:ARG:NH1	1:A:217:ILE:HG23	2.23	0.54
1:J:160:SER:HB3	1:J:166:GLN:HE22	1.72	0.54
1:J:172:ARG:HD2	1:J:221:ILE:CG1	2.39	0.53
1:J:162:ASN:OD1	1:J:164:SER:HB3	2.09	0.53
1:J:49:THR:OG1	1:J:196:THR:HG22	2.09	0.53
1:A:172:ARG:HD2	1:A:221:ILE:CG1	2.39	0.52
1:A:42:MET:HE1	1:A:206:PRO:HG2	1.91	0.52
1:J:119:SER:HB2	1:J:122:GLU:CG	2.35	0.52
1:G:55:ASN:HB3	4:G:256:HOH:O	2.09	0.52
1:G:17:ILE:HD13	1:G:228:ARG:HD3	1.91	0.52
1:A:88:TRP:HB3	1:A:217:ILE:HD11	1.92	0.51
1:G:88:TRP:HB3	1:G:217:ILE:HD11	1.91	0.51
1:J:116:LYS:HG3	1:J:188:VAL:HB	1.92	0.51
1:D:172:ARG:HD2	1:D:221:ILE:CG1	2.41	0.51
1:A:172:ARG:HD2	1:A:221:ILE:HG13	1.93	0.51
1:A:118:ASN:HA	1:A:187:VAL:HG21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:HB3	1:A:166:GLN:HE21	1.76	0.51
1:J:23:PRO:HB2	1:J:40:TRP:O	2.10	0.51
1:A:96:SER:OG	1:A:230:LEU:HA	2.12	0.50
1:D:183:GLU:HB3	1:D:186:ALA:HB2	1.94	0.49
1:J:51:HIS:HB2	1:J:64:VAL:HG23	1.95	0.49
1:A:119:SER:HB2	1:A:122:GLU:CG	2.38	0.49
1:A:56:SER:HB3	1:A:189:ALA:O	2.13	0.49
1:J:100:TYR:HB2	1:J:207:ALA:CB	2.43	0.49
1:D:160:SER:HB3	1:D:166:GLN:HE21	1.73	0.49
1:G:87:GLU:HG3	1:G:182:TRP:O	2.13	0.48
1:D:51:HIS:HB2	1:D:64:VAL:HG23	1.95	0.48
1:G:45:GLY:HA2	1:G:200:LYS:HG3	1.95	0.48
1:J:158:ARG:NH1	1:J:158:ARG:HG3	2.29	0.48
1:G:96:SER:OG	1:G:230:LEU:HA	2.13	0.48
1:G:156:LEU:O	1:G:171:GLY:HA3	2.13	0.48
1:D:4:ILE:HD13	1:D:215:SER:HB3	1.95	0.47
1:G:118:ASN:ND2	1:G:185:SER:O	2.47	0.47
1:D:14:ASN:O	1:D:19:ASP:HB2	2.14	0.47
1:J:172:ARG:NH2	4:J:251:HOH:O	2.45	0.47
1:D:172:ARG:HD2	1:D:221:ILE:HG13	1.96	0.47
1:D:122:GLU:OE1	1:D:122:GLU:HA	2.15	0.47
1:G:170:VAL:HG22	1:G:226:THR:HG22	1.97	0.47
1:G:90:ARG:NH1	1:G:217:ILE:HG23	2.30	0.47
1:A:208:ASP:OD1	1:A:227:GLY:HA2	2.15	0.47
1:G:91:VAL:HG12	1:G:214:ILE:HG12	1.95	0.47
1:D:49:THR:OG1	1:D:196:THR:HG22	2.15	0.47
1:G:14:ASN:O	1:G:19:ASP:HB2	2.14	0.47
1:D:42:MET:CE	1:D:206:PRO:HG3	2.44	0.47
1:D:111:PHE:CE2	1:D:113:SER:HB2	2.50	0.47
1:D:51:HIS:O	1:D:63:ALA:HA	2.14	0.47
1:J:102:GLU:HG2	1:J:207:ALA:O	2.15	0.47
1:D:20:PRO:HB2	1:D:22:TYR:CZ	2.50	0.47
1:A:156:LEU:O	1:A:171:GLY:HA3	2.15	0.46
1:D:201:SER:O	1:D:203:ASP:O	2.34	0.46
1:D:122:GLU:OE1	1:D:122:GLU:CA	2.63	0.46
1:J:96:SER:OG	1:J:230:LEU:HA	2.16	0.46
1:A:137:GLN:HG2	1:A:140:LEU:CD1	2.45	0.46
1:G:52:ILE:O	1:G:192:ASP:HA	2.15	0.46
1:D:3:THR:O	1:D:215:SER:HA	2.16	0.46
1:G:3:THR:O	1:G:215:SER:HA	2.17	0.45
1:A:11:THR:O	1:A:205:HIS:HE1	2.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:TYR:CE1	1:G:176:TYR:CE1	3.04	0.45
1:J:112:THR:O	1:J:191:PHE:HA	2.17	0.45
1:D:211:ALA:CB	1:D:232:LEU:HD11	2.47	0.44
1:A:133:PHE:HA	1:A:137:GLN:OE1	2.18	0.44
1:D:126:LEU:CD2	1:D:179:VAL:HG22	2.48	0.44
1:D:119:SER:HB2	1:D:122:GLU:HG2	2.00	0.44
1:J:100:TYR:HB2	1:J:207:ALA:HB3	2.00	0.43
1:J:25:ILE:HD12	1:J:65:VAL:CG2	2.36	0.43
1:G:20:PRO:HB2	1:G:22:TYR:CE1	2.53	0.43
1:A:57:VAL:HG23	1:A:188:VAL:HG13	2.00	0.43
1:A:106:ILE:HB	1:A:154:LEU:HB3	2.00	0.43
1:D:126:LEU:HD23	1:D:179:VAL:HG22	2.01	0.43
1:G:9:LEU:HD11	1:G:65:VAL:HG22	2.01	0.43
1:D:105:THR:O	1:D:197:PHE:HA	2.18	0.43
1:G:172:ARG:HD2	1:G:221:ILE:CG1	2.44	0.43
1:J:139:ASP:O	1:J:176:TYR:HB2	2.19	0.43
1:G:92:GLY:HA2	1:G:109:TRP:CH2	2.54	0.43
1:D:187:VAL:HG12	1:D:188:VAL:HG23	2.00	0.42
1:D:43:GLN:HE21	1:D:46:LYS:HG3	1.84	0.42
1:A:133:PHE:HB3	1:A:148:THR:HB	2.01	0.42
1:J:111:PHE:CE2	1:J:113:SER:HB2	2.55	0.42
1:J:117:SER:O	1:J:119:SER:N	2.52	0.42
1:J:111:PHE:HB3	1:J:128:PHE:CZ	2.55	0.42
1:J:174:LEU:HD12	1:J:174:LEU:N	2.35	0.42
1:J:108:SER:HA	1:J:130:PHE:O	2.18	0.42
1:D:124:ASN:HA	1:G:129:MET:O	2.20	0.42
1:D:117:SER:HA	1:D:186:ALA:HA	2.02	0.42
1:J:133:PHE:HB3	1:J:148:THR:HB	2.02	0.42
1:G:20:PRO:HB2	1:G:22:TYR:CZ	2.55	0.42
1:A:207:ALA:HA	1:A:208:ASP:HA	1.94	0.41
1:J:20:PRO:HB2	1:J:22:TYR:CZ	2.55	0.41
1:G:211:ALA:CB	1:G:232:LEU:HD11	2.50	0.41
1:D:133:PHE:HB3	1:D:148:THR:HB	2.00	0.41
1:G:102:GLU:HB2	1:G:199:ILE:HG23	2.02	0.41
1:A:23:PRO:HB2	1:A:40:TRP:O	2.20	0.41
1:A:170:VAL:HG11	1:A:231:GLY:HA2	2.03	0.41
1:A:17:ILE:HD13	1:A:228:ARG:HD3	2.02	0.41
1:D:12:TYR:HA	1:D:13:PRO:HD3	1.82	0.41
1:G:14:ASN:C	1:G:19:ASP:HB2	2.41	0.41
1:G:111:PHE:CE2	1:G:113:SER:HB2	2.55	0.41
1:D:208:ASP:OD1	1:D:227:GLY:HA2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:O	1:A:215:SER:HA	2.21	0.41
1:A:205:HIS:ND1	1:A:206:PRO:HD2	2.36	0.41
1:J:162:ASN:C	1:J:162:ASN:OD1	2.59	0.41
1:G:118:ASN:N	1:G:118:ASN:ND2	2.63	0.41
1:D:135:LYS:HE2	1:D:135:LYS:HB3	1.70	0.41
1:D:52:ILE:O	1:D:192:ASP:HA	2.21	0.41
1:J:156:LEU:O	1:J:171:GLY:HA3	2.21	0.41
1:G:207:ALA:HA	1:G:208:ASP:HA	1.86	0.40
1:J:207:ALA:HA	1:J:208:ASP:HA	1.80	0.40
1:D:181:ILE:HD12	1:D:181:ILE:HA	1.76	0.40
1:G:170:VAL:HG13	1:G:226:THR:HA	2.04	0.40
1:A:55:ASN:OD1	1:A:57:VAL:N	2.49	0.40
1:J:55:ASN:OD1	1:J:57:VAL:N	2.53	0.40
1:D:91:VAL:HG12	1:D:214:ILE:HG12	2.03	0.40
1:G:28:ASP:HB3	1:G:31:SER:O	2.21	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	235/237 (99%)	219 (93%)	13 (6%)	3 (1%)	15	15
1	D	235/237 (99%)	219 (93%)	13 (6%)	3 (1%)	15	15
1	G	235/237 (99%)	225 (96%)	8 (3%)	2 (1%)	21	24
1	J	235/237 (99%)	222 (94%)	11 (5%)	2 (1%)	21	24
All	All	940/948 (99%)	885 (94%)	45 (5%)	10 (1%)	17	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	D	120	THR
1	D	203	ASP
1	G	120	THR
1	D	150	THR
1	J	118	ASN
1	A	120	THR
1	A	122	GLU
1	J	120	THR
1	G	118	ASN

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	202/202 (100%)	193 (96%)	9 (4%)	34	46
1	D	202/202 (100%)	189 (94%)	13 (6%)	22	28
1	G	202/202 (100%)	189 (94%)	13 (6%)	22	28
1	J	202/202 (100%)	181 (90%)	21 (10%)	9	10
All	All	808/808 (100%)	752 (93%)	56 (7%)	19	24

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	69	ASN
1	A	71	ASP
1	A	99	LEU
1	A	118	ASN
1	A	119	SER
1	A	123	THR
1	A	170	VAL
1	A	200	LYS
1	D	64	VAL
1	D	101	LYS
1	D	116	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	118	ASN
1	D	121	HIS
1	D	122	GLU
1	D	150	THR
1	D	161	SER
1	D	164	SER
1	D	170	VAL
1	D	181	ILE
1	D	198	LEU
1	D	228	ARG
1	G	9	LEU
1	G	39	LYS
1	G	64	VAL
1	G	99	LEU
1	G	113	SER
1	G	116	LYS
1	G	132	GLN
1	G	135	LYS
1	G	161	SER
1	G	164	SER
1	G	170	VAL
1	G	200	LYS
1	G	228	ARG
1	J	36	LYS
1	J	56	SER
1	J	64	VAL
1	J	82	ASP
1	J	99	LEU
1	J	101	LYS
1	J	116	LYS
1	J	120	THR
1	J	122	GLU
1	J	132	GLN
1	J	150	THR
1	J	151	ASP
1	J	158	ARG
1	J	164	SER
1	J	168	SER
1	J	170	VAL
1	J	172	ARG
1	J	188	VAL
1	J	198	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	223	SER
1	J	228	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	43	GLN
1	A	132	GLN
1	A	166	GLN
1	D	21	ASN
1	D	43	GLN
1	D	118	ASN
1	D	132	GLN
1	D	166	GLN
1	G	21	ASN
1	G	43	GLN
1	G	118	ASN
1	G	121	HIS
1	G	132	GLN
1	J	121	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	A	237/237 (100%)	-0.28	17 (7%)	18 26	8, 15, 39, 63	0
1	D	237/237 (100%)	-0.31	15 (6%)	23 31	8, 15, 40, 59	0
1	G	237/237 (100%)	-0.18	11 (4%)	36 45	10, 20, 41, 58	0
1	J	237/237 (100%)	-0.14	15 (6%)	23 31	8, 18, 41, 57	0
All	All	948/948 (100%)	-0.23	58 (6%)	25 33	8, 18, 41, 63	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	121	HIS	7.2
1	J	121	HIS	6.4
1	A	184	SER	6.1
1	J	118	ASN	6.0
1	D	121	HIS	5.9
1	A	121	HIS	5.8
1	G	120	THR	5.8
1	D	185	SER	5.6
1	D	120	THR	5.6
1	A	118	ASN	5.5
1	G	1	ALA	5.4
1	J	120	THR	5.3
1	A	1	ALA	5.3
1	G	185	SER	5.3
1	J	185	SER	5.3
1	A	185	SER	5.2
1	A	119	SER	5.0
1	G	118	ASN	4.8
1	G	69	ASN	4.7
1	A	120	THR	4.7
1	J	1	ALA	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	118	ASN	4.5
1	G	119	SER	4.1
1	A	69	ASN	4.0
1	A	122	GLU	3.9
1	J	184	SER	3.7
1	A	117	SER	3.2
1	J	162	ASN	3.1
1	A	161	SER	3.0
1	J	161	SER	3.0
1	D	184	SER	3.0
1	D	161	SER	2.9
1	D	16	ASP	2.9
1	D	69	ASN	2.9
1	J	119	SER	2.9
1	J	69	ASN	2.7
1	J	122	GLU	2.7
1	D	119	SER	2.6
1	A	189	ALA	2.5
1	J	186	ALA	2.5
1	A	82	ASP	2.5
1	D	122	GLU	2.5
1	D	203	ASP	2.5
1	D	1	ALA	2.4
1	G	161	SER	2.4
1	J	99	LEU	2.4
1	G	223	SER	2.4
1	D	186	ALA	2.3
1	J	163	GLY	2.3
1	D	117	SER	2.2
1	A	135	LYS	2.2
1	G	117	SER	2.2
1	A	16	ASP	2.1
1	G	151	ASP	2.1
1	D	41	ASN	2.1
1	A	186	ALA	2.1
1	A	162	ASN	2.0
1	J	41	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	J	240	1/1	0.99	0.04	-2.33	18,18,18,18	0
3	CA	G	240	1/1	0.99	0.04	-2.53	17,17,17,17	0
3	CA	D	240	1/1	1.00	0.04	-2.59	11,11,11,11	0
3	CA	A	240	1/1	0.99	0.04	-3.10	11,11,11,11	0
2	MN	J	239	1/1	0.99	0.03	-4.20	17,17,17,17	0
2	MN	D	239	1/1	1.00	0.02	-5.25	13,13,13,13	0
2	MN	A	239	1/1	1.00	0.03	-6.67	13,13,13,13	0
2	MN	G	239	1/1	1.00	0.03	-8.86	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.