WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 04:19 PM EST

PDB ID	:	1CAU
Title	:	DETERMINATION OF THREE CRYSTAL STRUCTURES OF CANAVALIN BY MOLECULAR REPLACEMENT
Authors	:	Ko, T-P.; Ng, J.D.; Day, J.; Greenwood, A.; McPherson, A.
Deposited on	:	1993-07-08
Resolution	:	2.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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

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	Percentile Ranks	Value
Clashscore		42
Ramachandran outliers		5.5%
Sidechain outliers		29.0%
RSRZ outliers		0.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
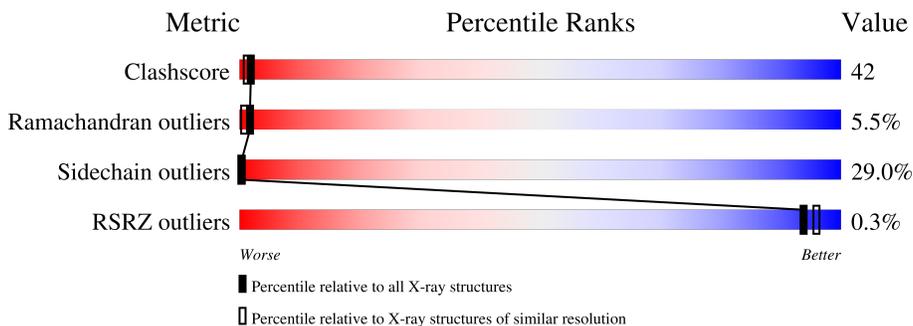
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	181	35% 38% 23% •
2	B	184	% 24% 46% 22% 7%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2930 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	181	Total	C	N	O	S	0	0	0
			1480	946	251	281	2			

- Molecule 2 is a protein called CANAVALIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1450	902	255	289	4			

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: CANAVALIN

Chain A:
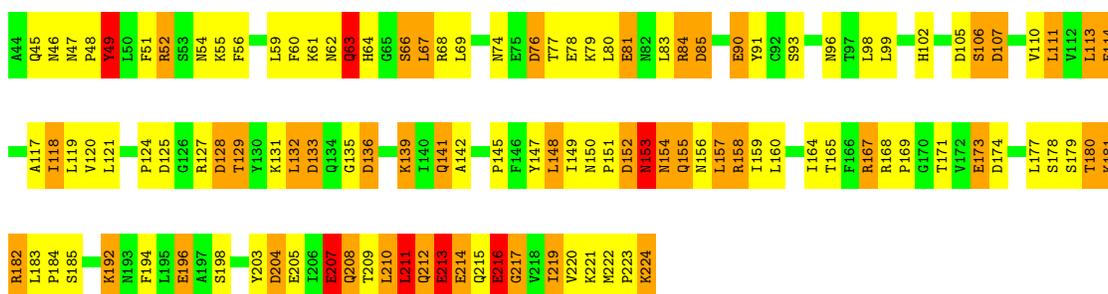
• Molecule 2: CANAVALIN

Chain B:
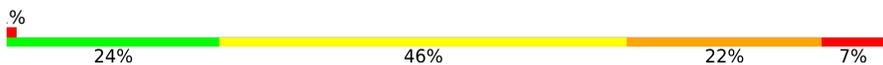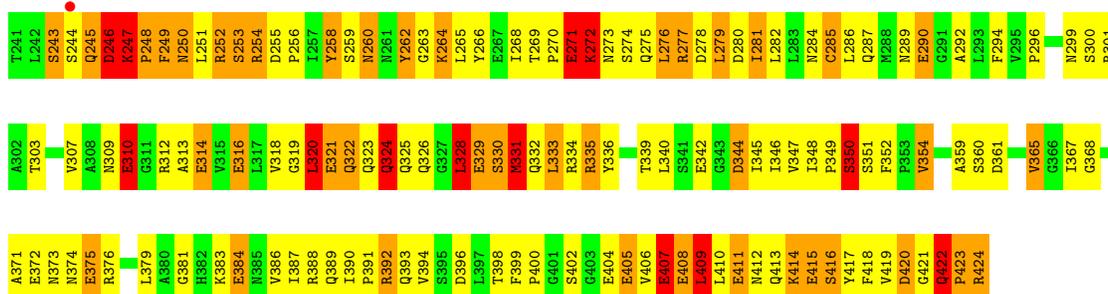
4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	106.00Å 106.00Å 106.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 28.33 – 2.02	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.30) 54.0 (28.33-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.29 (at 2.03Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.192 , (Not available) 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 149.0	EDS
L-test for twinning [2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.059 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2930	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 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	1.29	11/1511 (0.7%)	1.72	37/2046 (1.8%)
2	B	1.33	18/1472 (1.2%)	1.67	33/1992 (1.7%)
All	All	1.31	29/2983 (1.0%)	1.69	70/4038 (1.7%)

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	A	2	0
2	B	1	0
All	All	3	0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	290	GLU	CD-OE1	7.57	1.33	1.25
2	B	329	GLU	CD-OE1	7.52	1.33	1.25
1	A	213	GLU	CD-OE1	7.07	1.33	1.25
1	A	114	GLU	CD-OE1	6.97	1.33	1.25
1	A	196	GLU	CD-OE1	6.93	1.33	1.25
2	B	271	GLU	CD-OE2	6.92	1.33	1.25
2	B	407	GLU	CD-OE2	6.82	1.33	1.25
1	A	90	GLU	CD-OE2	6.79	1.33	1.25
1	A	81	GLU	CD-OE2	6.76	1.33	1.25
1	A	205	GLU	CD-OE2	6.73	1.33	1.25
2	B	310	GLU	CD-OE2	6.69	1.33	1.25
1	A	78	GLU	CD-OE2	6.54	1.32	1.25
2	B	342	GLU	CD-OE1	6.43	1.32	1.25
2	B	375	GLU	CD-OE2	6.39	1.32	1.25
2	B	408	GLU	CD-OE2	6.37	1.32	1.25
1	A	173	GLU	CD-OE1	6.31	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CD-OE1	6.00	1.32	1.25
2	B	404	GLU	CG-CD	5.84	1.60	1.51
2	B	248	PRO	N-CA	-5.78	1.37	1.47
2	B	411	GLU	CD-OE1	5.75	1.31	1.25
2	B	314	GLU	CD-OE2	5.71	1.31	1.25
1	A	49	TYR	N-CA	5.64	1.57	1.46
2	B	321	GLU	CD-OE2	5.64	1.31	1.25
2	B	384	GLU	CD-OE1	5.63	1.31	1.25
1	A	214	GLU	CD-OE1	5.55	1.31	1.25
2	B	316	GLU	CD-OE1	5.54	1.31	1.25
2	B	404	GLU	CB-CG	5.42	1.62	1.52
2	B	372	GLU	CD-OE1	5.34	1.31	1.25
2	B	415	GLU	CD-OE2	5.32	1.31	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	ASN	C-N-CD	-16.17	85.02	120.60
2	B	247	LYS	C-N-CD	-11.89	94.44	120.60
2	B	344	ASP	CB-CG-OD1	-9.78	109.50	118.30
2	B	376	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	136	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	A	125	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	A	133	ASP	CB-CG-OD1	7.75	125.27	118.30
1	A	136	ASP	CB-CG-OD1	7.68	125.21	118.30
2	B	278	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	124	PRO	N-CA-CB	7.67	112.50	103.30
2	B	422	GLN	C-N-CD	-7.43	104.24	120.60
1	A	85	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	128	ASP	CB-CG-OD2	-7.14	111.87	118.30
2	B	376	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	222	MET	C-N-CD	-7.04	105.11	120.60
2	B	330	SER	N-CA-CB	6.97	120.95	110.50
2	B	400	PRO	N-CA-C	-6.90	94.17	112.10
1	A	127	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	133	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	207	GLU	N-CA-CB	-6.72	98.51	110.60
2	B	331	MET	N-CA-CB	6.71	122.68	110.60
2	B	246	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	A	85	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	107	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	B	392	ARG	NE-CZ-NH1	6.47	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	328	LEU	N-CA-CB	6.38	123.15	110.40
1	A	76	ASP	CB-CG-OD1	-6.34	112.60	118.30
2	B	344	ASP	CB-CG-OD2	6.23	123.91	118.30
2	B	280	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	105	ASP	CB-CG-OD2	6.17	123.85	118.30
2	B	420	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	204	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	A	49	TYR	N-CA-C	6.11	127.50	111.00
2	B	258	TYR	N-CA-CB	6.05	121.49	110.60
1	A	63	GLN	N-CA-CB	6.04	121.46	110.60
1	A	52	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	128	ASP	CB-CG-OD1	5.95	123.65	118.30
2	B	324	GLN	C-N-CA	5.94	136.55	121.70
1	A	211	LEU	N-CA-C	5.94	127.04	111.00
2	B	255	ASP	CB-CG-OD2	5.85	123.56	118.30
2	B	320	LEU	N-CA-C	-5.81	95.30	111.00
2	B	407	GLU	N-CA-CB	5.79	121.03	110.60
2	B	278	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	204	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	214	GLU	N-CA-CB	5.58	120.65	110.60
2	B	252	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	54	ASN	CB-CA-C	-5.54	99.31	110.40
2	B	246	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	167	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	B	342	GLU	N-CA-CB	5.50	120.49	110.60
1	A	127	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	B	420	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	174	ASP	CB-CG-OD2	-5.45	113.40	118.30
2	B	415	GLU	N-CA-CB	5.44	120.39	110.60
2	B	254	ARG	NE-CZ-NH1	5.39	122.99	120.30
2	B	277	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	153	ASN	N-CA-C	5.33	125.38	111.00
1	A	81	GLU	N-CA-CB	5.27	120.08	110.60
1	A	52	ARG	N-CA-CB	5.24	120.03	110.60
2	B	409	LEU	CB-CA-C	5.21	120.10	110.20
1	A	107	ASP	N-CA-CB	5.20	119.96	110.60
1	A	153	ASN	CA-C-N	-5.17	105.82	117.20
1	A	105	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	B	342	GLU	CB-CA-C	5.11	120.62	110.40
2	B	336	TYR	CB-CG-CD1	-5.08	117.95	121.00
2	B	351	SER	N-CA-C	5.08	124.72	111.00
1	A	152	ASP	CB-CG-OD1	-5.06	113.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	THR	CA-CB-CG2	-5.04	105.34	112.40
2	B	280	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	A	125	ASP	CB-CG-OD1	5.00	122.81	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	63	GLN	CA
1	A	218	VAL	CA
2	B	242	LEU	CA

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	1480	0	1473	130	0
2	B	1450	0	1425	134	0
All	All	2930	0	2898	247	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 42.

All (247) 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:B:268:ILE:HG23	2:B:272:LYS:HD3	1.23	1.20
1:A:63:GLN:HE21	1:A:63:GLN:CA	1.60	1.13
1:A:63:GLN:HA	1:A:63:GLN:NE2	1.55	1.11
1:A:67:LEU:HD23	1:A:68:ARG:N	1.74	1.02
2:B:282:LEU:HD23	2:B:371:ALA:HB1	1.40	1.01
1:A:60:PHE:HA	1:A:182:ARG:HH12	1.22	0.98
1:A:155:GLN:HG2	1:A:156:ASN:H	1.35	0.92
1:A:63:GLN:HE21	1:A:63:GLN:HA	0.78	0.92
2:B:260:ASN:N	2:B:260:ASN:HD22	1.63	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD11	1:A:159:ILE:HG13	1.55	0.88
1:A:60:PHE:HA	1:A:182:ARG:NH1	1.88	0.88
2:B:282:LEU:HD23	2:B:371:ALA:CB	2.03	0.87
2:B:268:ILE:HG23	2:B:272:LYS:CD	2.04	0.84
1:A:114:GLU:HB3	1:A:158:ARG:HB3	1.58	0.83
1:A:61:LYS:HG3	1:A:66:SER:OG	1.80	0.81
2:B:303:THR:HG23	2:B:349:PRO:HA	1.63	0.80
1:A:67:LEU:HD23	1:A:67:LEU:C	2.01	0.79
2:B:268:ILE:CG2	2:B:272:LYS:HD3	2.10	0.79
2:B:272:LYS:O	2:B:272:LYS:HG2	1.83	0.78
2:B:323:GLN:C	2:B:325:GLN:H	1.86	0.77
1:A:114:GLU:HB2	1:A:158:ARG:HH11	1.50	0.76
2:B:299:ASN:HB3	2:B:374:ASN:OD1	1.86	0.76
2:B:320:LEU:HD23	2:B:333:LEU:HB3	1.66	0.76
1:A:80:LEU:HD22	1:A:83:LEU:HD12	1.66	0.75
2:B:318:VAL:HG12	2:B:319:GLY:N	2.01	0.75
2:B:258:TYR:HB3	2:B:417:TYR:CD2	2.20	0.75
2:B:323:GLN:OE1	2:B:326:GLN:HA	1.86	0.75
1:A:114:GLU:HB3	1:A:158:ARG:CB	2.16	0.74
1:A:154:ASN:OD1	1:A:154:ASN:N	2.20	0.74
2:B:409:LEU:O	2:B:412:ASN:HB2	1.88	0.74
1:A:120:VAL:HG22	1:A:129:THR:HG23	1.68	0.73
2:B:250:ASN:N	2:B:250:ASN:OD1	2.20	0.73
1:A:151:PRO:O	1:A:153:ASN:HB2	1.88	0.73
1:A:157:LEU:HD11	1:A:159:ILE:CG1	2.19	0.73
1:A:114:GLU:CB	1:A:158:ARG:HB3	2.18	0.72
2:B:381:GLY:HA2	2:B:413:GLN:HG3	1.71	0.72
1:A:120:VAL:HG11	1:A:147:TYR:OH	1.90	0.72
1:A:118:ILE:HG22	1:A:149:ILE:HB	1.72	0.70
1:A:132:LEU:HD23	2:B:250:ASN:HD22	1.55	0.70
1:A:181:LYS:O	1:A:182:ARG:HG2	1.92	0.70
1:A:111:LEU:HD23	1:A:111:LEU:N	2.07	0.70
2:B:248:PRO:HB3	2:B:275:GLN:CD	2.10	0.70
2:B:335:ARG:HH11	2:B:335:ARG:HG2	1.57	0.69
1:A:83:LEU:HD11	2:B:347:VAL:HG11	1.73	0.69
2:B:265:LEU:HD12	2:B:285:CYS:O	1.92	0.69
2:B:260:ASN:N	2:B:260:ASN:ND2	2.36	0.69
2:B:303:THR:HG23	2:B:348:ILE:O	1.93	0.69
1:A:157:LEU:CD1	1:A:159:ILE:HG13	2.23	0.69
1:A:74:ASN:OD1	1:A:74:ASN:N	2.26	0.68
1:A:81:GLU:O	1:A:84:ARG:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:CG	1:A:171:THR:HB	2.24	0.68
2:B:323:GLN:O	2:B:326:GLN:HG2	1.94	0.68
2:B:335:ARG:HG2	2:B:335:ARG:NH1	2.07	0.68
2:B:313:ALA:O	2:B:339:THR:HA	1.94	0.68
1:A:64:HIS:NE2	1:A:216:GLU:HG3	2.09	0.67
1:A:155:GLN:HG2	1:A:156:ASN:N	2.10	0.66
2:B:402:SER:OG	2:B:405:GLU:HB2	1.94	0.66
1:A:168:ARG:HG2	1:A:171:THR:HB	1.77	0.66
1:A:49:TYR:CE1	1:A:79:LYS:HE3	2.30	0.66
1:A:46:ASN:ND2	1:A:76:ASP:OD1	2.28	0.65
2:B:321:GLU:HG3	2:B:352:PHE:HZ	1.61	0.65
1:A:114:GLU:OE1	1:A:158:ARG:NH1	2.30	0.65
1:A:117:ALA:HB2	1:A:157:LEU:HD22	1.77	0.65
1:A:151:PRO:O	1:A:153:ASN:N	2.30	0.65
2:B:316:GLU:OE2	2:B:335:ARG:NH2	2.28	0.65
1:A:85:ASP:OD1	1:A:169:PRO:HB3	1.97	0.64
2:B:325:GLN:HB3	2:B:331:MET:N	2.12	0.63
2:B:269:THR:CG2	2:B:270:PRO:HD2	2.28	0.63
1:A:106:SER:C	1:A:142:ALA:HB2	2.18	0.63
2:B:318:VAL:HG12	2:B:319:GLY:H	1.62	0.63
1:A:62:ASN:ND2	1:A:216:GLU:OE1	2.31	0.62
1:A:49:TYR:CD1	1:A:79:LYS:HE3	2.33	0.62
1:A:181:LYS:HZ3	1:A:214:GLU:C	2.02	0.62
2:B:252:ARG:O	2:B:253:SER:HB3	1.99	0.62
1:A:67:LEU:C	1:A:67:LEU:CD2	2.68	0.62
2:B:279:LEU:HB3	2:B:281:ILE:HG13	1.80	0.62
2:B:398:THR:HB	2:B:399:PHE:CD1	2.36	0.61
1:A:160:LEU:CD1	2:B:307:VAL:HG21	2.31	0.61
2:B:256:PRO:HD3	2:B:266:TYR:CE1	2.35	0.61
2:B:269:THR:HG23	2:B:270:PRO:HD2	1.82	0.61
1:A:155:GLN:CG	1:A:156:ASN:H	2.12	0.60
1:A:151:PRO:C	1:A:153:ASN:H	2.04	0.60
2:B:258:TYR:HB3	2:B:417:TYR:HD2	1.66	0.59
1:A:62:ASN:OD1	1:A:64:HIS:N	2.27	0.59
2:B:328:LEU:HB3	2:B:329:GLU:OE1	2.03	0.59
2:B:323:GLN:O	2:B:323:GLN:HG3	2.02	0.59
1:A:160:LEU:HD11	2:B:307:VAL:HG21	1.84	0.59
1:A:51:PHE:O	2:B:346:ILE:HA	2.03	0.59
2:B:381:GLY:HA2	2:B:413:GLN:CG	2.32	0.58
1:A:139:LYS:HE2	1:A:141:GLN:OE1	2.02	0.58
2:B:266:TYR:O	2:B:284:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:VAL:HA	2:B:334:ARG:O	2.04	0.58
1:A:210:LEU:HD23	1:A:211:LEU:HB2	1.84	0.58
2:B:276:LEU:O	2:B:279:LEU:N	2.35	0.58
1:A:60:PHE:CA	1:A:182:ARG:HH12	2.07	0.57
2:B:393:GLN:O	2:B:393:GLN:HG3	2.02	0.57
1:A:81:GLU:O	1:A:81:GLU:HG3	2.05	0.56
1:A:102:HIS:O	1:A:145:PRO:HA	2.05	0.56
2:B:424:ARG:O	2:B:424:ARG:HG2	2.04	0.56
2:B:303:THR:CG2	2:B:349:PRO:HA	2.33	0.56
2:B:414:LYS:CD	2:B:414:LYS:H	2.17	0.56
1:A:113:LEU:HD22	2:B:365:VAL:HG21	1.86	0.55
2:B:318:VAL:HG13	2:B:334:ARG:O	2.07	0.55
2:B:259:SER:C	2:B:260:ASN:HD22	2.10	0.55
2:B:322:GLN:HB3	2:B:325:GLN:OE1	2.06	0.55
1:A:49:TYR:CG	1:A:79:LYS:NZ	2.74	0.55
2:B:318:VAL:CG1	2:B:319:GLY:N	2.70	0.55
1:A:220:VAL:HG12	1:A:220:VAL:O	2.08	0.54
1:A:62:ASN:OD1	1:A:62:ASN:C	2.46	0.54
1:A:149:ILE:O	1:A:151:PRO:HD3	2.08	0.54
1:A:168:ARG:HG2	1:A:171:THR:CB	2.38	0.54
2:B:312:ARG:HB3	2:B:359:ALA:HB3	1.90	0.54
1:A:49:TYR:CB	1:A:79:LYS:HZ2	2.20	0.54
1:A:52:ARG:HG3	2:B:340:LEU:HD11	1.89	0.54
1:A:59:LEU:HD12	1:A:67:LEU:HD22	1.90	0.54
1:A:61:LYS:H	1:A:182:ARG:HH22	1.55	0.54
2:B:259:SER:HA	2:B:263:GLY:O	2.08	0.54
2:B:335:ARG:HH11	2:B:335:ARG:CG	2.19	0.54
1:A:81:GLU:OE2	1:A:84:ARG:NH1	2.41	0.53
2:B:258:TYR:CD1	2:B:417:TYR:CE2	2.96	0.53
2:B:340:LEU:HG	2:B:344:ASP:CB	2.38	0.53
1:A:80:LEU:HD22	1:A:83:LEU:CD1	2.37	0.53
1:A:56:PHE:CD1	1:A:56:PHE:N	2.76	0.53
1:A:181:LYS:N	1:A:181:LYS:CD	2.72	0.53
2:B:249:PHE:N	2:B:249:PHE:CD1	2.73	0.52
1:A:210:LEU:HD23	1:A:211:LEU:HD23	1.91	0.52
1:A:216:GLU:OE1	1:A:216:GLU:HA	2.09	0.52
1:A:141:GLN:OE1	1:A:141:GLN:HA	2.09	0.52
2:B:268:ILE:HG12	2:B:272:LYS:HE2	1.90	0.52
1:A:63:GLN:HE21	1:A:63:GLN:C	2.10	0.51
2:B:325:GLN:CB	2:B:331:MET:HB2	2.40	0.51
1:A:216:GLU:O	1:A:219:ILE:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD13	1:A:148:LEU:HG	1.92	0.51
2:B:325:GLN:HB2	2:B:331:MET:HB2	1.93	0.51
1:A:132:LEU:HD23	2:B:250:ASN:ND2	2.25	0.50
1:A:135:GLY:O	2:B:252:ARG:HG3	2.12	0.50
2:B:256:PRO:HD3	2:B:266:TYR:HE1	1.76	0.50
2:B:262:TYR:N	2:B:262:TYR:CD1	2.80	0.49
2:B:268:ILE:HG23	2:B:272:LYS:CE	2.42	0.49
1:A:157:LEU:HD11	1:A:159:ILE:CD1	2.41	0.49
1:A:77:THR:HG23	1:A:80:LEU:H	1.77	0.49
2:B:262:TYR:HA	2:B:289:ASN:HD22	1.78	0.49
2:B:390:ILE:HG23	2:B:394:VAL:CG1	2.41	0.49
1:A:79:LYS:HE2	2:B:321:GLU:HB2	1.95	0.49
1:A:223:PRO:CD	1:A:224:LYS:H	2.25	0.49
2:B:249:PHE:O	2:B:275:GLN:NE2	2.45	0.49
2:B:296:PRO:HA	2:B:354:VAL:O	2.12	0.49
2:B:398:THR:CG2	2:B:399:PHE:CE1	2.95	0.49
2:B:418:PHE:O	2:B:419:VAL:HG23	2.12	0.49
1:A:49:TYR:CD1	1:A:79:LYS:CE	2.96	0.49
1:A:164:ILE:N	1:A:164:ILE:HD12	2.27	0.49
2:B:294:PHE:HD1	2:B:417:TYR:O	1.96	0.49
1:A:62:ASN:OD1	1:A:63:GLN:N	2.46	0.49
1:A:49:TYR:CD1	1:A:79:LYS:NZ	2.79	0.48
1:A:181:LYS:N	1:A:181:LYS:HD2	2.27	0.48
1:A:223:PRO:CG	1:A:224:LYS:H	2.26	0.48
1:A:135:GLY:C	2:B:252:ARG:HG3	2.33	0.48
1:A:158:ARG:NH2	2:B:309:ASN:ND2	2.61	0.48
1:A:59:LEU:O	1:A:182:ARG:NH1	2.47	0.48
2:B:391:PRO:O	2:B:394:VAL:N	2.34	0.48
1:A:114:GLU:HB2	1:A:158:ARG:NH1	2.24	0.48
1:A:132:LEU:CD2	2:B:250:ASN:ND2	2.77	0.47
1:A:136:ASP:HA	2:B:252:ARG:HB2	1.95	0.47
1:A:56:PHE:HB3	1:A:68:ARG:HB3	1.96	0.47
1:A:110:VAL:C	1:A:111:LEU:HD23	2.34	0.47
1:A:63:GLN:CA	1:A:63:GLN:NE2	2.34	0.47
2:B:246:ASP:O	2:B:247:LYS:HD3	2.15	0.47
2:B:316:GLU:O	2:B:354:VAL:HA	2.14	0.47
2:B:322:GLN:HB3	2:B:322:GLN:HE21	1.46	0.47
1:A:64:HIS:HD2	1:A:219:ILE:O	1.97	0.47
1:A:179:SER:OG	1:A:185:SER:N	2.45	0.47
2:B:323:GLN:O	2:B:326:GLN:N	2.48	0.47
1:A:68:ARG:NH2	1:A:90:GLU:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HB	1:A:217:GLY:HA2	1.96	0.47
2:B:344:ASP:N	2:B:344:ASP:OD1	2.47	0.46
1:A:83:LEU:HD11	2:B:347:VAL:CG1	2.44	0.46
1:A:132:LEU:CD2	2:B:250:ASN:HD22	2.26	0.46
1:A:196:GLU:OE2	1:A:203:TYR:HB2	2.15	0.46
2:B:269:THR:HG22	2:B:270:PRO:N	2.31	0.46
2:B:314:GLU:OE2	2:B:359:ALA:HB2	2.16	0.46
1:A:220:VAL:O	1:A:221:LYS:C	2.54	0.46
1:A:223:PRO:HD2	1:A:224:LYS:O	2.15	0.46
2:B:279:LEU:HB3	2:B:281:ILE:HB	1.98	0.46
1:A:114:GLU:HB3	1:A:158:ARG:HB2	1.96	0.46
1:A:204:ASP:O	1:A:208:GLN:HG3	2.16	0.46
1:A:49:TYR:CB	1:A:79:LYS:NZ	2.79	0.45
2:B:289:ASN:O	2:B:290:GLU:C	2.53	0.45
1:A:207:GLU:O	1:A:210:LEU:HB3	2.16	0.45
2:B:303:THR:O	2:B:368:GLY:HA2	2.15	0.45
1:A:119:LEU:HD12	1:A:147:TYR:O	2.16	0.45
2:B:324:GLN:C	2:B:325:GLN:OE1	2.55	0.45
1:A:150:ASN:OD1	1:A:155:GLN:O	2.34	0.45
1:A:223:PRO:HG2	1:A:224:LYS:O	2.17	0.45
2:B:282:LEU:CD2	2:B:371:ALA:HB1	2.29	0.45
2:B:391:PRO:O	2:B:394:VAL:HB	2.16	0.45
2:B:398:THR:HB	2:B:399:PHE:HD1	1.79	0.44
1:A:212:GLN:NE2	1:A:214:GLU:HB2	2.32	0.44
2:B:299:ASN:O	2:B:350:SER:O	2.35	0.44
2:B:325:GLN:HB2	2:B:331:MET:CB	2.47	0.44
2:B:387:ILE:HG22	2:B:410:LEU:HD11	2.00	0.44
2:B:309:ASN:C	2:B:310:GLU:HG2	2.38	0.44
1:A:211:LEU:HD13	1:A:212:GLN:N	2.32	0.44
2:B:273:ASN:OD1	2:B:274:SER:N	2.51	0.44
1:A:181:LYS:NZ	1:A:215:GLN:HA	2.33	0.43
1:A:181:LYS:NZ	1:A:215:GLN:N	2.66	0.43
1:A:215:GLN:H	1:A:215:GLN:HG3	1.62	0.43
1:A:91:TYR:CZ	1:A:93:SER:HB2	2.53	0.43
1:A:192:LYS:NZ	1:A:192:LYS:HB3	2.31	0.43
2:B:273:ASN:O	2:B:277:ARG:HB2	2.18	0.43
1:A:49:TYR:HB3	1:A:79:LYS:NZ	2.33	0.43
2:B:258:TYR:CD1	2:B:417:TYR:CD2	3.06	0.43
2:B:263:GLY:HA2	2:B:287:GLN:O	2.19	0.43
2:B:406:VAL:O	2:B:407:GLU:C	2.55	0.43
2:B:345:ILE:HG22	2:B:346:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:ASP:OD1	2:B:421:GLY:O	2.38	0.42
1:A:118:ILE:CG2	1:A:149:ILE:HB	2.44	0.42
2:B:332:GLN:H	2:B:332:GLN:HG3	1.61	0.42
1:A:51:PHE:O	2:B:346:ILE:HG13	2.19	0.42
1:A:98:LEU:HD12	1:A:148:LEU:O	2.19	0.42
2:B:269:THR:CG2	2:B:270:PRO:CD	2.97	0.42
1:A:182:ARG:O	1:A:183:LEU:HD12	2.20	0.42
2:B:262:TYR:HB3	2:B:292:ALA:CB	2.50	0.42
2:B:275:GLN:O	2:B:279:LEU:HD22	2.20	0.42
1:A:211:LEU:HD13	1:A:211:LEU:C	2.40	0.42
2:B:383:LYS:N	2:B:416:SER:OG	2.53	0.41
1:A:96:ASN:O	1:A:221:LYS:HA	2.21	0.41
1:A:181:LYS:HZ1	1:A:215:GLN:HA	1.85	0.41
2:B:307:VAL:O	2:B:307:VAL:HG12	2.17	0.41
2:B:387:ILE:C	2:B:389:GLN:H	2.22	0.41
2:B:320:LEU:H	2:B:320:LEU:HG	1.56	0.41
2:B:345:ILE:CG2	2:B:346:ILE:N	2.84	0.41
2:B:325:GLN:CB	2:B:331:MET:CB	2.99	0.41
2:B:335:ARG:O	2:B:335:ARG:HG3	2.07	0.41
1:A:211:LEU:HA	1:A:211:LEU:HD22	1.31	0.41
1:A:118:ILE:HD13	1:A:151:PRO:HG3	2.02	0.41
1:A:213:GLU:O	1:A:215:GLN:HG3	2.21	0.41
2:B:258:TYR:CG	2:B:417:TYR:CD2	3.09	0.41
2:B:322:GLN:N	2:B:331:MET:SD	2.82	0.41
2:B:386:VAL:O	2:B:389:GLN:HB2	2.20	0.41
1:A:212:GLN:OE1	1:A:213:GLU:N	2.50	0.40
2:B:269:THR:HG22	2:B:270:PRO:CD	2.50	0.40
2:B:323:GLN:HG3	2:B:326:GLN:NE2	2.36	0.40
2:B:422:GLN:HA	2:B:423:PRO:HD2	1.79	0.40
2:B:245:GLN:HG2	2:B:249:PHE:HD2	1.86	0.40
2:B:259:SER:HB2	2:B:264:LYS:HG3	2.04	0.40
2:B:318:VAL:CG1	2:B:319:GLY:H	2.30	0.40
2:B:270:PRO:HB3	2:B:277:ARG:HA	2.03	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	179/181 (99%)	146 (82%)	26 (14%)	7 (4%)	3	1
2	B	182/184 (99%)	143 (79%)	26 (14%)	13 (7%)	1	0
All	All	361/365 (99%)	289 (80%)	52 (14%)	20 (6%)	2	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	TYR
1	A	152	ASP
1	A	153	ASN
1	A	184	PRO
2	B	247	LYS
2	B	253	SER
2	B	350	SER
2	B	423	PRO
1	A	182	ARG
1	A	217	GLY
2	B	246	ASP
2	B	272	LYS
2	B	388	ARG
2	B	408	GLU
1	A	48	PRO
2	B	243	SER
2	B	271	GLU
2	B	324	GLN
2	B	422	GLN
2	B	392	ARG

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	167/167 (100%)	121 (72%)	46 (28%)	0	0
2	B	161/161 (100%)	112 (70%)	49 (30%)	0	0
All	All	328/328 (100%)	233 (71%)	95 (29%)	0	0

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	55	LYS
1	A	63	GLN
1	A	66	SER
1	A	67	LEU
1	A	69	LEU
1	A	84	ARG
1	A	99	LEU
1	A	106	SER
1	A	107	ASP
1	A	111	LEU
1	A	113	LEU
1	A	118	ILE
1	A	121	LEU
1	A	128	ASP
1	A	129	THR
1	A	131	LYS
1	A	132	LEU
1	A	133	ASP
1	A	139	LYS
1	A	141	GLN
1	A	148	LEU
1	A	153	ASN
1	A	154	ASN
1	A	155	GLN
1	A	157	LEU
1	A	158	ARG
1	A	167	ARG
1	A	173	GLU
1	A	177	LEU
1	A	178	SER

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Mol	Chain	Res	Type
1	A	180	THR
1	A	181	LYS
1	A	192	LYS
1	A	194	PHE
1	A	198	SER
1	A	207	GLU
1	A	208	GLN
1	A	209	THR
1	A	210	LEU
1	A	211	LEU
1	A	212	GLN
1	A	213	GLU
1	A	216	GLU
1	A	219	ILE
1	A	224	LYS
2	B	243	SER
2	B	244	SER
2	B	245	GLN
2	B	246	ASP
2	B	247	LYS
2	B	249	PHE
2	B	250	ASN
2	B	251	LEU
2	B	254	ARG
2	B	260	ASN
2	B	262	TYR
2	B	264	LYS
2	B	271	GLU
2	B	272	LYS
2	B	276	LEU
2	B	279	LEU
2	B	281	ILE
2	B	285	CYS
2	B	286	LEU
2	B	300	SER
2	B	301	ARG
2	B	310	GLU
2	B	320	LEU
2	B	322	GLN
2	B	324	GLN
2	B	328	LEU
2	B	330	SER

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Mol	Chain	Res	Type
2	B	331	MET
2	B	333	LEU
2	B	335	ARG
2	B	350	SER
2	B	354	VAL
2	B	360	SER
2	B	361	ASP
2	B	365	VAL
2	B	367	ILE
2	B	373	ASN
2	B	375	GLU
2	B	379	LEU
2	B	384	GLU
2	B	396	ASP
2	B	405	GLU
2	B	407	GLU
2	B	409	LEU
2	B	411	GLU
2	B	414	LYS
2	B	415	GLU
2	B	416	SER
2	B	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	116	GLN
1	A	150	ASN
1	A	193	ASN
1	A	208	GLN
2	B	260	ASN
2	B	284	ASN
2	B	289	ASN
2	B	309	ASN
2	B	322	GLN
2	B	332	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

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(Å²)	Q<0.9
1	A	181/181 (100%)	-0.56	0	100	100	8, 20, 31, 37	0
2	B	184/184 (100%)	-0.49	1 (0%)	91	94	10, 19, 31, 36	0
All	All	365/365 (100%)	-0.52	1 (0%)	94	96	8, 20, 31, 37	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	244	SER	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.