



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:14 AM UTC

PDB ID : 1CAV / pdb_00001cav
Title : THE THREE-DIMENSIONAL STRUCTURE OF CANAVALIN FROM
JACK BEAN (CANAVALLIA ENSIFORMIS)
Authors : Ko, T-P.; Ng, J.D.; McPherson, A.
Deposited on : 1993-05-27
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

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

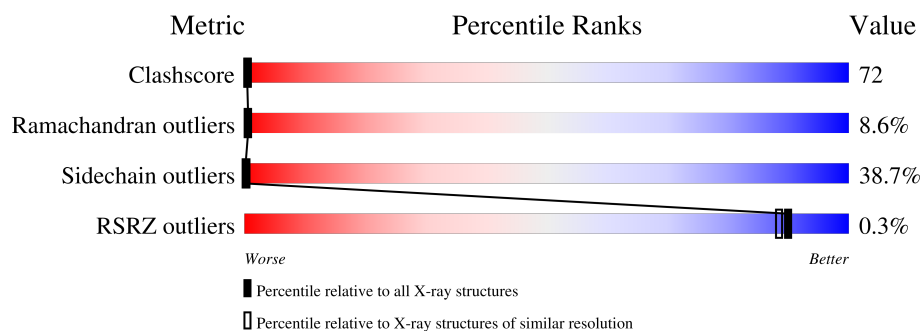
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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	181	 19% 36% 30% 14%
2	B	184	 16% 42% 28% 15%

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			

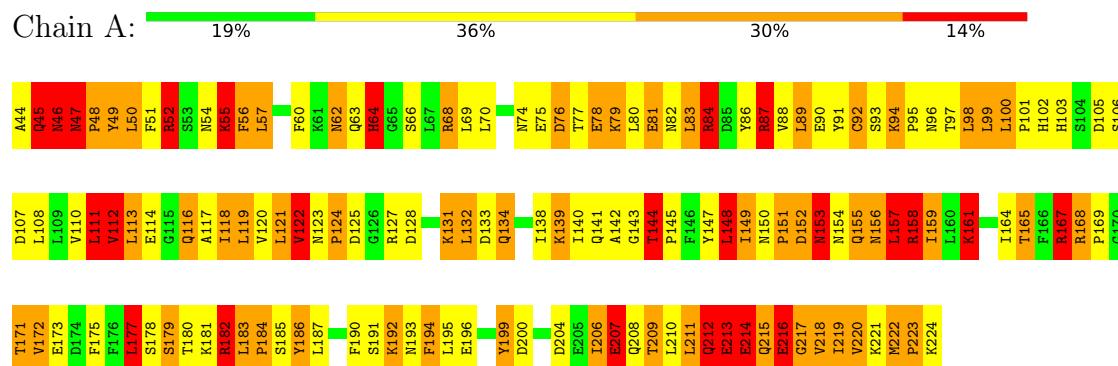
- Molecule 2 is a protein called CANAVALIN.

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

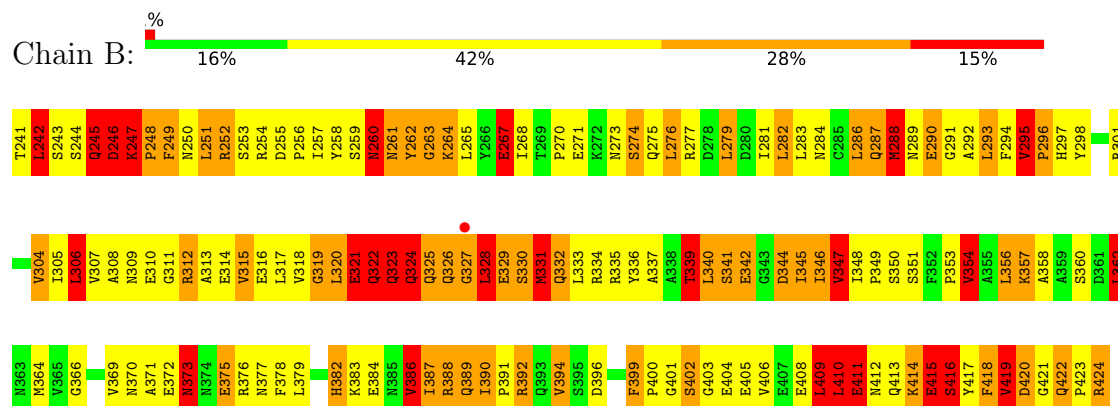
3 Residue-property plots

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 2: CANAVALIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	126.35Å 126.35Å 51.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 68.7 (8.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.51Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.188 , (Not available) 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 167.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	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 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	1.55	7/1511 (0.5%)	1.99	67/2046 (3.3%)
2	B	1.71	23/1472 (1.6%)	2.08	59/1992 (3.0%)
All	All	1.63	30/2983 (1.0%)	2.03	126/4038 (3.1%)

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	4	2
2	B	2	0
All	All	6	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	319	GLY	CA-C	9.01	1.60	1.52
2	B	253	SER	N-CA	8.10	1.56	1.45
1	A	52	ARG	NE-CZ	7.14	1.41	1.33
2	B	252	ARG	C-N	6.53	1.42	1.33
2	B	250	ASN	C-N	6.50	1.42	1.33
1	A	144	THR	CA-C	-6.27	1.45	1.53
2	B	328	LEU	N-CA	6.22	1.54	1.46
1	A	221	LYS	CA-C	-6.19	1.45	1.52
1	A	128	ASP	N-CA	-6.17	1.38	1.46
2	B	319	GLY	N-CA	6.09	1.50	1.45
2	B	356	LEU	C-N	-6.01	1.25	1.33
2	B	340	LEU	CA-C	-5.98	1.45	1.53
2	B	375	GLU	C-N	-5.78	1.25	1.33
2	B	248	PRO	N-CA	-5.67	1.40	1.47
2	B	327	GLY	N-CA	5.42	1.53	1.45
2	B	263	GLY	CA-C	5.40	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	326	GLN	CA-C	5.37	1.60	1.53
2	B	251	LEU	CA-C	5.32	1.59	1.52
1	A	87	ARG	CA-C	-5.32	1.46	1.52
2	B	390	ILE	N-CA	-5.32	1.40	1.47
2	B	327	GLY	C-N	5.30	1.41	1.33
2	B	252	ARG	N-CA	5.27	1.52	1.46
2	B	322	GLN	N-CA	5.23	1.52	1.46
1	A	200	ASP	CG-OD1	5.12	1.35	1.25
2	B	308	ALA	CA-C	-5.12	1.46	1.52
2	B	290	GLU	CD-OE1	5.08	1.35	1.25
2	B	249	PHE	N-CA	-5.08	1.39	1.46
1	A	165	THR	CA-C	5.07	1.60	1.53
2	B	420	ASP	CA-C	-5.01	1.46	1.52
2	B	251	LEU	C-N	5.00	1.40	1.33

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	324	GLN	N-CA-C	-11.54	94.80	111.30
2	B	247	LYS	CA-C-N	10.74	133.27	119.84
2	B	247	LYS	C-N-CA	10.74	133.27	119.84
1	A	154	ASN	N-CA-C	-10.39	98.19	112.12
1	A	214	GLU	N-CA-C	-10.08	92.30	108.73
1	A	153	ASN	CA-C-N	9.69	137.09	122.17
1	A	153	ASN	C-N-CA	9.69	137.09	122.17
1	A	46	ASN	N-CA-C	8.71	129.35	110.80
2	B	246	ASP	N-CA-C	8.69	129.31	110.80
2	B	305	ILE	CA-C-N	-8.65	110.79	122.99
2	B	305	ILE	C-N-CA	-8.65	110.79	122.99
2	B	294	PHE	N-CA-C	-8.64	96.02	109.25
2	B	419	VAL	N-CA-CB	-8.42	97.34	111.23
1	A	220	VAL	N-CA-CB	-8.36	100.82	112.52
2	B	247	LYS	C-N-CD	-8.35	90.75	125.00
2	B	260	ASN	CA-CB-CG	8.31	120.91	112.60
1	A	75	GLU	N-CA-C	8.23	124.16	111.56
2	B	319	GLY	CA-C-N	8.18	134.30	122.44
2	B	319	GLY	C-N-CA	8.18	134.30	122.44
2	B	319	GLY	N-CA-C	8.12	122.95	111.10
2	B	386	VAL	CB-CA-C	8.10	118.19	111.06
2	B	244	SER	N-CA-C	-8.00	103.42	113.02
2	B	399	PHE	CA-C-N	7.57	129.30	119.84
2	B	399	PHE	C-N-CA	7.57	129.30	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLN	N-CA-CB	7.51	121.59	109.28
1	A	94	LYS	CA-C-N	7.34	127.39	119.90
1	A	94	LYS	C-N-CA	7.34	127.39	119.90
1	A	149	ILE	CB-CA-C	-7.33	99.20	110.50
1	A	161	LYS	N-CA-CB	7.30	122.18	110.65
2	B	373	ASN	N-CA-C	7.23	126.19	110.80
2	B	362	LEU	N-CA-C	7.17	121.52	109.76
2	B	321	GLU	N-CA-C	7.10	125.93	110.80
1	A	78	GLU	N-CA-C	-7.08	104.25	113.17
2	B	420	ASP	N-CA-CB	7.02	121.74	110.16
1	A	153	ASN	N-CA-C	7.00	125.70	110.80
1	A	216	GLU	N-CA-C	-6.96	95.98	110.80
1	A	50	LEU	N-CA-CB	6.96	121.85	110.37
1	A	144	THR	CB-CA-C	-6.95	99.05	109.26
2	B	245	GLN	CA-C-N	6.74	134.42	121.54
2	B	245	GLN	C-N-CA	6.74	134.42	121.54
2	B	350	SER	N-CA-C	6.50	124.65	110.80
2	B	276	LEU	N-CA-C	-6.48	105.95	114.31
2	B	420	ASP	CA-CB-CG	-6.47	106.13	112.60
1	A	155	GLN	CB-CA-C	6.46	119.05	110.06
2	B	402	SER	N-CA-C	6.44	118.33	108.42
2	B	390	ILE	N-CA-C	-6.43	101.95	108.96
2	B	322	GLN	N-CA-C	6.34	118.86	108.52
2	B	331	MET	N-CA-CB	6.33	119.12	110.38
1	A	121	LEU	CA-C-N	-6.30	114.99	122.93
1	A	121	LEU	C-N-CA	-6.30	114.99	122.93
1	A	215	GLN	CB-CA-C	6.26	122.87	110.42
2	B	344	ASP	N-CA-C	6.25	118.62	110.43
2	B	409	LEU	CA-C-N	6.24	128.89	120.65
2	B	409	LEU	C-N-CA	6.24	128.89	120.65
2	B	306	LEU	N-CA-CB	6.23	121.14	110.68
2	B	373	ASN	CA-CB-CG	-6.19	106.41	112.60
1	A	216	GLU	CA-C-N	6.19	133.54	121.41
1	A	216	GLU	C-N-CA	6.19	133.54	121.41
2	B	253	SER	N-CA-C	6.15	118.52	109.24
2	B	382	HIS	CA-CB-CG	-6.14	107.66	113.80
1	A	50	LEU	CB-CA-C	6.14	120.60	110.78
1	A	45	GLN	CA-C-N	6.13	133.26	121.54
1	A	45	GLN	C-N-CA	6.13	133.26	121.54
1	A	112	VAL	N-CA-C	6.02	117.07	107.98
1	A	183	LEU	CB-CA-C	-6.01	102.29	110.22
2	B	326	GLN	N-CA-C	6.00	119.67	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASP	N-CA-C	-5.96	98.68	108.76
1	A	153	ASN	O-C-N	5.96	130.51	122.59
1	A	194	PHE	N-CA-CB	5.92	118.94	110.06
1	A	151	PRO	CA-C-N	5.85	132.72	121.54
1	A	151	PRO	C-N-CA	5.85	132.72	121.54
1	A	212	GLN	CA-C-N	5.82	131.23	123.20
1	A	212	GLN	C-N-CA	5.82	131.23	123.20
1	A	214	GLU	N-CA-CB	5.80	119.88	110.42
1	A	194	PHE	O-C-N	5.80	128.27	122.12
1	A	157	LEU	N-CA-C	5.79	118.17	108.73
2	B	248	PRO	CA-C-N	5.79	129.09	120.87
2	B	248	PRO	C-N-CA	5.79	129.09	120.87
1	A	149	ILE	N-CA-C	5.77	117.05	108.46
2	B	288	MET	N-CA-C	5.75	117.92	109.24
2	B	247	LYS	O-C-N	5.74	127.92	121.32
2	B	415	GLU	CA-C-N	5.71	132.46	121.54
2	B	415	GLU	C-N-CA	5.71	132.46	121.54
1	A	204	ASP	CB-CA-C	5.69	120.24	110.79
1	A	158	ARG	N-CA-CB	5.66	119.58	110.65
1	A	213	GLU	N-CA-C	5.62	116.46	108.54
2	B	305	ILE	CB-CA-C	-5.59	104.19	110.96
2	B	295	VAL	N-CA-CB	-5.56	103.42	111.21
1	A	122	VAL	N-CA-C	5.54	116.28	108.36
1	A	47	ASN	CA-C-N	5.53	126.75	119.84
1	A	47	ASN	C-N-CA	5.53	126.75	119.84
1	A	148	LEU	CB-CA-C	5.53	120.60	109.38
1	A	199	TYR	N-CA-C	5.52	118.48	111.69
2	B	347	VAL	CB-CA-C	5.52	118.77	111.21
1	A	220	VAL	CA-C-N	-5.51	114.44	122.65
1	A	220	VAL	C-N-CA	-5.51	114.44	122.65
1	A	101	PRO	N-CA-CB	5.49	108.45	103.34
2	B	252	ARG	N-CA-C	5.46	122.43	110.80
1	A	64	HIS	CA-C-N	-5.39	112.82	120.97
1	A	64	HIS	C-N-CA	-5.39	112.82	120.97
1	A	103	HIS	CA-CB-CG	5.39	119.19	113.80
2	B	410	LEU	N-CA-C	5.38	116.84	110.97
1	A	128	ASP	CA-CB-CG	5.37	117.97	112.60
2	B	250	ASN	N-CA-C	5.37	117.46	110.43
2	B	416	SER	N-CA-C	5.35	122.20	110.80
2	B	249	PHE	N-CA-C	-5.35	102.37	110.28
2	B	267	GLU	N-CA-C	5.27	116.66	107.49
2	B	326	GLN	N-CA-CB	-5.26	103.92	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	GLN	CB-CG-CD	5.22	121.48	112.60
2	B	354	VAL	CB-CA-C	-5.20	101.40	110.71
1	A	151	PRO	N-CA-C	5.20	118.77	110.40
1	A	219	ILE	N-CA-CB	5.20	119.11	111.52
2	B	339	THR	N-CA-C	-5.19	100.05	108.41
1	A	111	LEU	CB-CA-C	5.12	118.62	109.65
2	B	411	GLU	N-CA-CB	5.12	117.89	110.47
2	B	242	LEU	N-CA-C	5.11	118.05	110.48
1	A	81	GLU	N-CA-CB	5.10	118.99	110.32
1	A	165	THR	N-CA-C	5.08	117.41	110.55
1	A	182	ARG	CA-C-N	5.07	130.37	122.26
1	A	182	ARG	C-N-CA	5.07	130.37	122.26
2	B	323	GLN	N-CA-CB	5.06	117.84	110.25
1	A	177	LEU	CA-C-N	5.06	128.88	120.94
1	A	177	LEU	C-N-CA	5.06	128.88	120.94
1	A	55	LYS	N-CA-C	5.02	116.49	107.80
1	A	207	GLU	CB-CG-CD	-5.02	104.07	112.60
1	A	186	TYR	N-CA-C	-5.01	105.89	111.36

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	46	ASN	CA
1	A	50	LEU	CA
1	A	75	GLU	CA
1	A	155	GLN	CA
2	B	246	ASP	CA
2	B	373	ASN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	GLU	Mainchain
1	A	62	ASN	Mainchain

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	234	1
2	B	1450	0	1425	199	1
All	All	2930	0	2898	417	1

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 72.

All (417) 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:A:139:LYS:HE3	1:A:141:GLN:HE22	1.03	1.18
1:A:49:TYR:CE2	2:B:321:GLU:HG3	1.79	1.15
1:A:114:GLU:HB3	1:A:158:ARG:HG3	1.27	1.08
2:B:331:MET:HE2	2:B:332:GLN:H	1.26	1.01
1:A:47:ASN:H	1:A:76:ASP:CB	1.76	0.98
2:B:248:PRO:HA	2:B:275:GLN:HE22	1.28	0.96
2:B:242:LEU:HD12	2:B:249:PHE:CE1	2.04	0.93
1:A:68:ARG:HG3	1:A:68:ARG:HH11	1.32	0.93
1:A:207:GLU:HA	1:A:210:LEU:HB3	1.48	0.92
1:A:139:LYS:HE3	1:A:141:GLN:NE2	1.84	0.92
2:B:262:TYR:OH	2:B:420:ASP:HB2	1.69	0.91
1:A:49:TYR:CG	1:A:79:LYS:HD2	2.05	0.90
1:A:207:GLU:HB3	1:A:210:LEU:HD22	1.54	0.89
2:B:288:MET:HE2	2:B:358:ALA:HB2	1.54	0.88
1:A:168:ARG:HB3	1:A:171:THR:HG21	1.56	0.88
1:A:207:GLU:HA	1:A:210:LEU:CB	2.03	0.88
1:A:49:TYR:HB3	1:A:79:LYS:CD	2.02	0.88
1:A:213:GLU:HG2	1:A:215:GLN:HE21	1.37	0.88
1:A:168:ARG:HB3	1:A:171:THR:CG2	2.04	0.88
1:A:79:LYS:NZ	2:B:322:GLN:HG3	1.87	0.88
1:A:122:VAL:HG22	1:A:145:PRO:HG2	1.56	0.87
1:A:190:PHE:HB2	1:A:195:LEU:HD21	1.56	0.87
2:B:416:SER:HB2	2:B:417:TYR:CD2	2.09	0.87
2:B:329:GLU:CD	2:B:329:GLU:H	1.82	0.86
1:A:213:GLU:CG	1:A:215:GLN:HE21	1.90	0.85
1:A:191:SER:OG	1:A:194:PHE:HB2	1.75	0.84
1:A:46:ASN:HA	1:A:76:ASP:HB3	1.60	0.84
1:A:47:ASN:H	1:A:76:ASP:HB2	1.42	0.84
1:A:94:LYS:HB3	1:A:95:PRO:HD2	1.57	0.84
1:A:114:GLU:CB	1:A:158:ARG:HG3	2.08	0.84
1:A:49:TYR:CD1	1:A:79:LYS:HD2	2.13	0.83
2:B:248:PRO:HA	2:B:275:GLN:NE2	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:O	1:A:217:GLY:N	2.13	0.82
2:B:331:MET:CE	2:B:332:GLN:H	1.94	0.81
1:A:157:LEU:HD12	1:A:158:ARG:N	1.97	0.80
1:A:49:TYR:CD2	2:B:321:GLU:HG3	2.17	0.80
1:A:60:PHE:HE1	1:A:219:ILE:HD12	1.47	0.80
2:B:408:GLU:HG3	2:B:409:LEU:N	1.97	0.79
1:A:192:LYS:HG3	1:A:193:ASN:H	1.49	0.78
1:A:49:TYR:HB3	1:A:79:LYS:HD2	1.65	0.77
1:A:47:ASN:H	1:A:76:ASP:HB3	1.48	0.77
1:A:46:ASN:CA	1:A:76:ASP:HB3	2.15	0.76
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.51	0.75
1:A:222:MET:HG2	1:A:223:PRO:HD2	1.68	0.75
2:B:420:ASP:OD2	2:B:422:GLN:HB3	1.86	0.75
2:B:331:MET:CE	2:B:332:GLN:HB2	2.16	0.74
2:B:340:LEU:HD21	2:B:346:ILE:HB	1.67	0.74
2:B:245:GLN:HG2	2:B:249:PHE:CE2	2.22	0.74
1:A:79:LYS:HZ1	2:B:322:GLN:HG3	1.50	0.73
2:B:408:GLU:HG3	2:B:409:LEU:H	1.51	0.73
2:B:378:PHE:CZ	2:B:417:TYR:HD1	2.07	0.73
2:B:414:LYS:CD	2:B:414:LYS:H	1.99	0.73
2:B:247:LYS:C	2:B:249:PHE:H	1.96	0.73
1:A:92:CYS:HA	1:A:157:LEU:O	1.89	0.72
2:B:322:GLN:O	2:B:325:GLN:HB3	1.90	0.72
1:A:79:LYS:NZ	2:B:321:GLU:HB3	2.05	0.72
1:A:49:TYR:CB	1:A:79:LYS:HD2	2.20	0.72
2:B:260:ASN:CG	2:B:261:ASN:H	1.97	0.72
1:A:213:GLU:HG2	1:A:215:GLN:NE2	2.05	0.72
2:B:412:ASN:C	2:B:414:LYS:HE2	2.15	0.72
2:B:347:VAL:O	2:B:348:ILE:HD13	1.89	0.71
2:B:412:ASN:O	2:B:414:LYS:HE2	1.91	0.71
2:B:408:GLU:CG	2:B:409:LEU:H	2.03	0.71
1:A:119:LEU:HD21	1:A:121:LEU:HG	1.72	0.70
1:A:212:GLN:OE1	1:A:213:GLU:N	2.21	0.70
2:B:424:ARG:HD3	2:B:424:ARG:N	2.07	0.70
2:B:325:GLN:OE1	2:B:331:MET:HA	1.91	0.70
1:A:51:PHE:O	2:B:346:ILE:HD12	1.93	0.69
2:B:362:LEU:HD23	2:B:364:MET:HG3	1.73	0.69
2:B:267:GLU:HB2	2:B:284:ASN:CB	2.23	0.69
1:A:84:ARG:HG3	1:A:84:ARG:NH1	2.08	0.68
1:A:62:ASN:OD1	1:A:64:HIS:N	2.21	0.68
1:A:60:PHE:CE1	1:A:219:ILE:HD12	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:GLU:CG	2:B:335:ARG:HD2	2.24	0.68
2:B:411:GLU:C	2:B:413:GLN:H	1.99	0.68
2:B:286:LEU:C	2:B:286:LEU:HD22	2.18	0.67
1:A:98:LEU:O	1:A:219:ILE:HA	1.93	0.67
1:A:164:ILE:N	1:A:164:ILE:HD12	2.10	0.67
1:A:62:ASN:OD1	1:A:62:ASN:C	2.37	0.67
1:A:87:ARG:NH1	1:A:87:ARG:HG3	2.10	0.67
1:A:56:PHE:HA	1:A:70:LEU:HA	1.76	0.67
2:B:310:GLU:HA	2:B:342:GLU:HG2	1.76	0.67
1:A:64:HIS:HA	1:A:94:LYS:HG3	1.76	0.67
1:A:151:PRO:O	1:A:153:ASN:N	2.26	0.67
1:A:213:GLU:CB	1:A:215:GLN:HE21	2.08	0.67
1:A:212:GLN:CD	1:A:213:GLU:N	2.53	0.66
2:B:243:SER:C	2:B:245:GLN:H	2.04	0.66
2:B:406:VAL:O	2:B:410:LEU:HG	1.96	0.66
2:B:267:GLU:HB2	2:B:284:ASN:HB3	1.77	0.65
2:B:262:TYR:CE1	2:B:420:ASP:HA	2.31	0.65
1:A:199:TYR:HB2	1:A:206:ILE:HD11	1.78	0.65
1:A:153:ASN:HB3	1:A:155:GLN:N	2.12	0.64
1:A:192:LYS:HG3	1:A:193:ASN:N	2.13	0.64
1:A:100:LEU:CD1	1:A:218:VAL:HA	2.28	0.64
1:A:57:LEU:N	1:A:69:LEU:O	2.31	0.64
1:A:111:LEU:C	1:A:111:LEU:HD12	2.22	0.64
2:B:320:LEU:HD12	2:B:332:GLN:O	1.98	0.64
2:B:408:GLU:CG	2:B:409:LEU:N	2.61	0.64
1:A:157:LEU:HD12	1:A:157:LEU:C	2.24	0.63
1:A:179:SER:OG	1:A:211:LEU:HA	1.99	0.63
1:A:56:PHE:HB3	1:A:69:LEU:C	2.23	0.63
1:A:164:ILE:HD12	1:A:164:ILE:H	1.63	0.63
1:A:68:ARG:HH11	1:A:68:ARG:CG	2.09	0.63
1:A:99:LEU:HD13	1:A:102:HIS:CE1	2.33	0.63
2:B:288:MET:HE2	2:B:358:ALA:CB	2.29	0.63
1:A:79:LYS:HZ2	2:B:321:GLU:HB3	1.62	0.63
2:B:313:ALA:O	2:B:340:LEU:N	2.30	0.63
1:A:208:GLN:O	1:A:209:THR:OG1	2.13	0.62
2:B:307:VAL:HG22	2:B:345:ILE:CG1	2.29	0.62
1:A:60:PHE:HE1	1:A:219:ILE:CD1	2.12	0.62
1:A:63:GLN:HB3	1:A:216:GLU:OE2	1.98	0.62
1:A:105:ASP:OD1	1:A:105:ASP:N	2.32	0.62
1:A:47:ASN:N	1:A:76:ASP:HB3	2.15	0.62
2:B:408:GLU:O	2:B:410:LEU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLN:NE2	1:A:214:GLU:N	2.48	0.61
1:A:114:GLU:HB3	1:A:158:ARG:CG	2.18	0.61
1:A:52:ARG:NH1	1:A:54:ASN:OD1	2.33	0.61
1:A:120:VAL:HG21	1:A:147:TYR:CE2	2.35	0.61
1:A:44:ALA:O	1:A:45:GLN:HB3	2.01	0.61
1:A:63:GLN:O	1:A:94:LYS:NZ	2.29	0.61
2:B:392:ARG:HD2	2:B:403:GLY:O	2.01	0.61
1:A:49:TYR:CE2	2:B:334:ARG:NH1	2.68	0.61
1:A:167:ARG:CG	1:A:167:ARG:HH11	2.14	0.61
1:A:168:ARG:HB3	1:A:171:THR:HG22	1.82	0.61
1:A:190:PHE:CB	1:A:195:LEU:HD21	2.29	0.61
1:A:213:GLU:HB3	1:A:215:GLN:HE21	1.64	0.61
2:B:274:SER:HA	2:B:277:ARG:HB3	1.82	0.60
2:B:316:GLU:HG3	2:B:335:ARG:HD2	1.82	0.60
1:A:120:VAL:HG21	1:A:147:TYR:CZ	2.37	0.60
2:B:242:LEU:HD12	2:B:249:PHE:HE1	1.64	0.60
1:A:167:ARG:HH11	1:A:167:ARG:HG3	1.66	0.60
1:A:207:GLU:HB3	1:A:210:LEU:CD2	2.30	0.60
2:B:251:LEU:HD13	2:B:268:ILE:HD13	1.83	0.60
1:A:212:GLN:HE21	1:A:214:GLU:CB	2.14	0.59
2:B:282:LEU:C	2:B:282:LEU:HD12	2.27	0.59
1:A:212:GLN:CD	1:A:213:GLU:C	2.70	0.59
2:B:301:ARG:NH2	2:B:370:ASN:ND2	2.51	0.59
2:B:419:VAL:HG13	2:B:420:ASP:N	2.17	0.59
1:A:49:TYR:HD2	2:B:336:TYR:OH	1.86	0.59
1:A:151:PRO:C	1:A:153:ASN:H	2.11	0.59
2:B:324:GLN:O	2:B:324:GLN:HG3	2.02	0.59
2:B:331:MET:CE	2:B:332:GLN:N	2.63	0.59
2:B:295:VAL:HG22	2:B:296:PRO:HD2	1.84	0.58
2:B:259:SER:HA	2:B:264:LYS:HB3	1.84	0.58
1:A:87:ARG:HG3	1:A:87:ARG:HH11	1.68	0.58
1:A:91:TYR:HB3	1:A:159:ILE:HG22	1.85	0.58
1:A:206:ILE:O	1:A:210:LEU:HB2	2.03	0.57
1:A:122:VAL:O	1:A:145:PRO:HD2	2.04	0.57
1:A:182:ARG:HD2	1:A:182:ARG:N	2.19	0.57
1:A:79:LYS:HZ1	2:B:321:GLU:C	2.13	0.57
1:A:48:PRO:O	1:A:77:THR:HA	2.05	0.57
2:B:288:MET:HE1	2:B:292:ALA:O	2.04	0.57
1:A:207:GLU:HA	1:A:210:LEU:HB2	1.83	0.56
2:B:270:PRO:HD3	2:B:281:ILE:O	2.05	0.56
2:B:297:HIS:O	2:B:353:PRO:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:HB3	1:A:79:LYS:CG	2.36	0.56
2:B:307:VAL:HG22	2:B:345:ILE:HG12	1.87	0.56
1:A:76:ASP:OD1	1:A:76:ASP:N	2.38	0.56
1:A:111:LEU:HD11	1:A:113:LEU:CD2	2.36	0.56
1:A:117:ALA:HB2	1:A:157:LEU:HD21	1.87	0.56
1:A:172:VAL:C	1:A:173:GLU:HG2	2.31	0.56
2:B:314:GLU:HB2	2:B:357:LYS:HB3	1.88	0.56
1:A:149:ILE:O	1:A:151:PRO:HD3	2.07	0.55
2:B:325:GLN:OE1	2:B:331:MET:HG2	2.06	0.55
1:A:179:SER:HB3	1:A:184:PRO:HB3	1.88	0.55
2:B:371:ALA:O	2:B:372:GLU:C	2.49	0.55
2:B:391:PRO:HD2	2:B:394:VAL:HG21	1.89	0.55
1:A:79:LYS:HZ2	2:B:322:GLN:HG3	1.71	0.55
2:B:415:GLU:HB3	2:B:419:VAL:CG2	2.37	0.55
2:B:420:ASP:OD1	2:B:421:GLY:N	2.40	0.55
1:A:79:LYS:O	1:A:80:LEU:HD23	2.06	0.55
1:A:111:LEU:HD11	1:A:113:LEU:HD21	1.89	0.55
2:B:315:VAL:HG23	2:B:356:LEU:CD1	2.36	0.55
2:B:319:GLY:O	2:B:333:LEU:HA	2.07	0.55
1:A:89:LEU:N	1:A:89:LEU:HD12	2.21	0.55
1:A:102:HIS:O	1:A:145:PRO:HA	2.07	0.55
2:B:306:LEU:HG	2:B:346:ILE:HG22	1.88	0.55
2:B:331:MET:HE2	2:B:332:GLN:HB2	1.88	0.54
2:B:281:ILE:HD13	2:B:369:VAL:HG12	1.89	0.54
2:B:315:VAL:O	2:B:337:ALA:HA	2.07	0.54
1:A:49:TYR:HE2	2:B:334:ARG:HH11	1.55	0.54
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.20	0.54
2:B:325:GLN:OE1	2:B:330:SER:O	2.25	0.54
2:B:358:ALA:HA	2:B:362:LEU:CD1	2.38	0.54
2:B:267:GLU:HB2	2:B:284:ASN:HB2	1.88	0.54
2:B:242:LEU:H	2:B:242:LEU:CD1	2.18	0.54
1:A:100:LEU:HD12	1:A:218:VAL:HG22	1.90	0.54
1:A:195:LEU:CD1	1:A:199:TYR:CE2	2.91	0.54
2:B:241:THR:CG2	2:B:249:PHE:CZ	2.92	0.53
2:B:242:LEU:CD1	2:B:249:PHE:CE1	2.84	0.53
2:B:248:PRO:CA	2:B:275:GLN:HE22	2.11	0.53
1:A:106:SER:OG	1:A:165:THR:HG22	2.09	0.53
1:A:148:LEU:HD11	1:A:159:ILE:HD13	1.89	0.53
1:A:212:GLN:CG	1:A:213:GLU:N	2.70	0.53
2:B:258:TYR:CD2	2:B:265:LEU:HD23	2.43	0.53
2:B:262:TYR:CZ	2:B:420:ASP:HB2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:HD12	2:B:242:LEU:H	1.73	0.53
1:A:112:VAL:HG21	1:A:132:LEU:HB3	1.90	0.53
2:B:258:TYR:O	2:B:264:LYS:HA	2.08	0.53
1:A:223:PRO:CG	1:A:224:LYS:H	2.22	0.53
1:A:222:MET:CG	1:A:223:PRO:HD2	2.39	0.52
2:B:271:GLU:OE2	2:B:372:GLU:HA	2.09	0.52
2:B:411:GLU:C	2:B:413:GLN:N	2.67	0.52
2:B:245:GLN:HG2	2:B:249:PHE:HE2	1.72	0.52
2:B:378:PHE:CE2	2:B:417:TYR:CD1	2.98	0.52
1:A:56:PHE:CD1	1:A:56:PHE:N	2.77	0.52
2:B:331:MET:HE1	2:B:332:GLN:HB2	1.89	0.52
2:B:346:ILE:HG13	2:B:348:ILE:HD11	1.92	0.52
1:A:222:MET:HG2	1:A:223:PRO:CD	2.39	0.52
1:A:219:ILE:C	1:A:220:VAL:HG23	2.34	0.52
2:B:246:ASP:O	2:B:246:ASP:OD1	2.28	0.52
1:A:167:ARG:CZ	1:A:167:ARG:HB3	2.40	0.52
2:B:241:THR:HA	2:B:249:PHE:CE1	2.45	0.52
1:A:87:ARG:HH11	1:A:87:ARG:CG	2.21	0.52
1:A:117:ALA:O	1:A:118:ILE:HD12	2.09	0.51
2:B:262:TYR:HH	2:B:420:ASP:HB2	1.72	0.51
1:A:74:ASN:OD1	1:A:84:ARG:HA	2.09	0.51
1:A:57:LEU:N	1:A:57:LEU:CD2	2.74	0.51
2:B:399:PHE:O	2:B:401:GLY:N	2.37	0.51
1:A:77:THR:OG1	1:A:79:LYS:HG3	2.11	0.51
2:B:281:ILE:CD1	2:B:369:VAL:HG12	2.41	0.51
2:B:306:LEU:HD13	2:B:364:MET:SD	2.49	0.51
1:A:56:PHE:N	1:A:56:PHE:HD1	2.09	0.51
2:B:292:ALA:O	2:B:293:LEU:C	2.53	0.51
1:A:47:ASN:N	1:A:76:ASP:CB	2.60	0.51
1:A:74:ASN:O	1:A:74:ASN:ND2	2.44	0.51
1:A:167:ARG:HB3	1:A:167:ARG:NH1	2.26	0.51
2:B:408:GLU:C	2:B:410:LEU:N	2.68	0.51
1:A:90:GLU:CG	1:A:91:TYR:N	2.74	0.51
2:B:313:ALA:O	2:B:339:THR:HA	2.11	0.50
1:A:68:ARG:HG3	1:A:68:ARG:NH1	2.10	0.50
1:A:86:TYR:HE1	1:A:164:ILE:HG23	1.76	0.50
1:A:212:GLN:NE2	1:A:214:GLU:CA	2.74	0.50
2:B:256:PRO:HG2	2:B:259:SER:HB2	1.93	0.50
2:B:298:TYR:CZ	2:B:377:ASN:HB2	2.47	0.50
2:B:260:ASN:OD1	2:B:262:TYR:N	2.44	0.50
2:B:402:SER:O	2:B:405:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:GLU:O	2:B:409:LEU:C	2.53	0.50
1:A:123:ASN:OD1	1:A:125:ASP:OD1	2.29	0.50
2:B:311:GLY:H	2:B:342:GLU:CG	2.24	0.50
2:B:325:GLN:CD	2:B:331:MET:HG2	2.36	0.50
1:A:89:LEU:HD22	1:A:161:LYS:CD	2.42	0.50
1:A:100:LEU:HD12	1:A:218:VAL:HA	1.93	0.49
2:B:306:LEU:HG	2:B:346:ILE:CG2	2.41	0.49
2:B:315:VAL:HG23	2:B:356:LEU:HD12	1.93	0.49
1:A:219:ILE:C	1:A:220:VAL:CG2	2.85	0.49
2:B:373:ASN:ND2	2:B:373:ASN:O	2.45	0.49
2:B:295:VAL:O	2:B:296:PRO:C	2.56	0.49
2:B:320:LEU:CD1	2:B:333:LEU:HD12	2.43	0.49
2:B:270:PRO:CG	2:B:371:ALA:HB1	2.43	0.49
1:A:155:GLN:HG3	1:A:156:ASN:N	2.28	0.49
1:A:89:LEU:HD22	1:A:161:LYS:HD3	1.93	0.49
2:B:298:TYR:O	2:B:298:TYR:CD1	2.67	0.48
2:B:323:GLN:OE1	2:B:325:GLN:HB3	2.13	0.48
2:B:346:ILE:CG2	2:B:346:ILE:O	2.61	0.48
2:B:307:VAL:HG22	2:B:345:ILE:HG13	1.95	0.48
1:A:86:TYR:CE1	1:A:164:ILE:HG23	2.49	0.48
2:B:291:GLY:HA2	2:B:357:LYS:HE3	1.95	0.48
1:A:172:VAL:O	1:A:173:GLU:HG2	2.14	0.48
1:A:110:VAL:HG21	1:A:140:ILE:CD1	2.43	0.48
2:B:324:GLN:O	2:B:324:GLN:CG	2.62	0.48
2:B:378:PHE:CZ	2:B:417:TYR:CD1	2.95	0.48
1:A:206:ILE:HG23	1:A:210:LEU:HD13	1.96	0.48
1:A:212:GLN:CD	1:A:214:GLU:N	2.72	0.48
2:B:331:MET:HE2	2:B:332:GLN:N	2.08	0.48
2:B:288:MET:HE3	2:B:292:ALA:HB3	1.96	0.47
1:A:57:LEU:N	1:A:57:LEU:HD22	2.28	0.47
1:A:118:ILE:N	1:A:118:ILE:CD1	2.76	0.47
1:A:118:ILE:HD13	1:A:151:PRO:HG3	1.96	0.47
1:A:122:VAL:O	1:A:144:THR:HG22	2.13	0.47
1:A:207:GLU:CA	1:A:210:LEU:HB3	2.32	0.47
1:A:212:GLN:HE21	1:A:214:GLU:HB2	1.79	0.47
1:A:118:ILE:N	1:A:118:ILE:HD13	2.30	0.47
2:B:273:ASN:O	2:B:277:ARG:HB2	2.15	0.47
1:A:215:GLN:O	1:A:216:GLU:C	2.56	0.47
2:B:241:THR:HG22	2:B:249:PHE:CZ	2.50	0.47
1:A:60:PHE:CZ	1:A:218:VAL:CG1	2.98	0.47
1:A:77:THR:HG1	1:A:79:LYS:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:HD22	2:B:287:GLN:N	2.30	0.47
2:B:301:ARG:CZ	2:B:370:ASN:HD21	2.27	0.47
2:B:341:SER:O	2:B:342:GLU:C	2.58	0.46
1:A:50:LEU:HD23	1:A:51:PHE:H	1.79	0.46
1:A:191:SER:OG	1:A:194:PHE:CB	2.58	0.46
2:B:251:LEU:CD1	2:B:268:ILE:CD1	2.93	0.46
1:A:119:LEU:C	1:A:119:LEU:HD23	2.40	0.46
2:B:301:ARG:CZ	2:B:370:ASN:ND2	2.79	0.46
2:B:378:PHE:CE2	2:B:417:TYR:CE1	3.03	0.46
1:A:111:LEU:CD1	1:A:113:LEU:HD23	2.45	0.46
2:B:270:PRO:HG3	2:B:371:ALA:CB	2.45	0.46
2:B:291:GLY:HA2	2:B:357:LYS:CE	2.46	0.46
2:B:415:GLU:HB3	2:B:419:VAL:HG22	1.97	0.46
1:A:120:VAL:CG2	1:A:147:TYR:CE2	2.98	0.46
1:A:193:ASN:OD1	1:A:194:PHE:N	2.49	0.46
1:A:94:LYS:CB	1:A:95:PRO:HD2	2.29	0.46
1:A:213:GLU:HB3	1:A:215:GLN:NE2	2.29	0.46
1:A:117:ALA:C	1:A:118:ILE:HD13	2.41	0.46
1:A:192:LYS:CG	1:A:193:ASN:N	2.78	0.46
2:B:289:ASN:O	2:B:290:GLU:C	2.59	0.46
1:A:167:ARG:NH1	1:A:167:ARG:CB	2.79	0.45
2:B:247:LYS:CB	2:B:248:PRO:CD	2.89	0.45
1:A:82:ASN:OD1	1:A:83:LEU:HD12	2.17	0.45
1:A:212:GLN:NE2	1:A:213:GLU:C	2.74	0.45
1:A:98:LEU:HD23	1:A:149:ILE:HG12	1.98	0.45
1:A:117:ALA:C	1:A:118:ILE:CD1	2.90	0.45
1:A:167:ARG:CG	1:A:167:ARG:NH1	2.78	0.45
1:A:195:LEU:CD1	1:A:199:TYR:HE2	2.29	0.45
1:A:110:VAL:CG2	1:A:140:ILE:HD12	2.46	0.45
1:A:195:LEU:HB3	1:A:206:ILE:HD13	1.98	0.45
1:A:66:SER:O	1:A:91:TYR:CD1	2.70	0.45
2:B:323:GLN:O	2:B:326:GLN:NE2	2.48	0.45
2:B:288:MET:HE2	2:B:288:MET:HB2	1.86	0.45
1:A:116:GLN:OE1	1:A:131:LYS:HG2	2.17	0.45
1:A:195:LEU:HD13	1:A:199:TYR:CE2	2.52	0.45
2:B:414:LYS:CD	2:B:414:LYS:N	2.73	0.45
1:A:164:ILE:N	1:A:164:ILE:CD1	2.77	0.45
2:B:388:ARG:HH11	2:B:388:ARG:HB3	1.82	0.45
2:B:389:GLN:HE21	2:B:389:GLN:HB2	1.35	0.45
1:A:99:LEU:CD2	1:A:218:VAL:CG1	2.95	0.45
2:B:251:LEU:HD13	2:B:268:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:TYR:CE1	2:B:420:ASP:CA	2.98	0.45
1:A:90:GLU:HG3	1:A:91:TYR:H	1.81	0.44
1:A:206:ILE:CG2	1:A:210:LEU:HD13	2.47	0.44
2:B:288:MET:CE	2:B:292:ALA:O	2.65	0.44
1:A:49:TYR:HB3	1:A:79:LYS:HG3	1.98	0.44
1:A:60:PHE:CZ	1:A:218:VAL:HG12	2.53	0.44
1:A:66:SER:O	1:A:91:TYR:HD1	2.01	0.44
1:A:79:LYS:NZ	2:B:321:GLU:CB	2.79	0.44
1:A:100:LEU:HD11	1:A:218:VAL:HA	1.97	0.44
1:A:177:LEU:HD13	1:A:177:LEU:HA	1.65	0.44
2:B:245:GLN:HB3	2:B:246:ASP:H	1.35	0.44
2:B:358:ALA:CB	2:B:362:LEU:HD13	2.48	0.44
1:A:190:PHE:CB	1:A:195:LEU:CD2	2.95	0.44
1:A:87:ARG:HD2	1:A:87:ARG:HA	1.64	0.44
1:A:89:LEU:HB2	1:A:161:LYS:HD2	1.99	0.44
1:A:93:SER:HB2	1:A:97:THR:OG1	2.17	0.44
1:A:111:LEU:HD12	1:A:113:LEU:HD23	2.00	0.44
1:A:177:LEU:O	1:A:185:SER:OG	2.28	0.44
2:B:260:ASN:CG	2:B:261:ASN:N	2.72	0.44
2:B:241:THR:HG23	2:B:249:PHE:CZ	2.53	0.44
1:A:213:GLU:HG2	1:A:215:GLN:HG2	1.99	0.44
2:B:289:ASN:O	2:B:291:GLY:N	2.51	0.44
1:A:49:TYR:HA	1:A:79:LYS:HG3	2.00	0.44
1:A:195:LEU:O	1:A:199:TYR:HB2	2.18	0.43
2:B:323:GLN:OE1	2:B:325:GLN:HG2	2.18	0.43
2:B:346:ILE:O	2:B:346:ILE:HG23	2.18	0.43
2:B:357:LYS:HD3	2:B:357:LYS:C	2.43	0.43
1:A:46:ASN:HA	1:A:76:ASP:CB	2.37	0.43
1:A:119:LEU:HG	1:A:120:VAL:N	2.34	0.43
1:A:179:SER:HA	1:A:184:PRO:HA	2.01	0.43
1:A:199:TYR:CB	1:A:206:ILE:HD11	2.47	0.43
2:B:254:ARG:HG3	2:B:255:ASP:H	1.84	0.43
1:A:49:TYR:HA	1:A:77:THR:OG1	2.18	0.43
1:A:60:PHE:CD1	1:A:60:PHE:C	2.96	0.43
1:A:95:PRO:HA	1:A:150:ASN:ND2	2.32	0.43
2:B:296:PRO:HA	2:B:354:VAL:O	2.18	0.43
2:B:258:TYR:CE2	2:B:265:LEU:HD23	2.53	0.43
1:A:55:LYS:O	1:A:55:LYS:HG3	2.18	0.43
2:B:413:GLN:O	2:B:413:GLN:HG3	2.17	0.43
1:A:49:TYR:CD2	2:B:321:GLU:CG	2.96	0.43
1:A:107:ASP:OD1	1:A:142:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:O	1:A:187:LEU:C	2.62	0.43
1:A:100:LEU:HD11	1:A:217:GLY:O	2.19	0.43
2:B:282:LEU:HD12	2:B:282:LEU:O	2.19	0.42
2:B:286:LEU:C	2:B:286:LEU:CD2	2.89	0.42
1:A:79:LYS:NZ	2:B:321:GLU:C	2.76	0.42
1:A:134:GLN:HE21	1:A:134:GLN:HB3	1.59	0.42
2:B:293:LEU:O	2:B:418:PHE:HA	2.19	0.42
2:B:419:VAL:CG1	2:B:420:ASP:N	2.80	0.42
2:B:247:LYS:CB	2:B:248:PRO:HD2	2.48	0.42
2:B:402:SER:OG	2:B:405:GLU:OE2	2.37	0.42
1:A:105:ASP:OD1	1:A:106:SER:N	2.52	0.42
2:B:257:ILE:O	2:B:258:TYR:CD1	2.73	0.42
2:B:281:ILE:HG22	2:B:282:LEU:N	2.34	0.42
2:B:301:ARG:NH2	2:B:370:ASN:HD21	2.18	0.42
2:B:378:PHE:HB2	2:B:384:GLU:O	2.20	0.42
2:B:387:ILE:HA	2:B:390:ILE:CD1	2.48	0.42
1:A:133:ASP:O	1:A:134:GLN:C	2.61	0.42
1:A:212:GLN:NE2	1:A:214:GLU:HG2	2.35	0.42
2:B:382:HIS:CD2	2:B:411:GLU:HB2	2.54	0.42
2:B:422:GLN:O	2:B:422:GLN:HG2	2.18	0.42
1:A:99:LEU:CD2	1:A:218:VAL:HG13	2.49	0.42
1:A:111:LEU:CD1	1:A:113:LEU:CD2	2.98	0.42
1:A:118:ILE:CD1	1:A:151:PRO:HG3	2.49	0.42
2:B:358:ALA:CB	2:B:362:LEU:CD1	2.98	0.42
1:A:49:TYR:HB3	1:A:79:LYS:HD3	1.97	0.42
2:B:279:LEU:HD13	2:B:279:LEU:HA	1.72	0.42
2:B:325:GLN:N	2:B:326:GLN:OE1	2.53	0.42
1:A:158:ARG:NH1	2:B:309:ASN:ND2	2.68	0.41
1:A:193:ASN:HA	1:A:196:GLU:HB2	2.01	0.41
2:B:242:LEU:O	2:B:249:PHE:CZ	2.72	0.41
2:B:312:ARG:HB2	2:B:360:SER:OG	2.20	0.41
1:A:179:SER:C	1:A:180:THR:HG23	2.45	0.41
2:B:284:ASN:O	2:B:366:GLY:N	2.46	0.41
1:A:64:HIS:HB3	1:A:97:THR:HG21	2.02	0.41
1:A:91:TYR:O	1:A:158:ARG:HA	2.20	0.41
2:B:276:LEU:C	2:B:279:LEU:H	2.29	0.41
2:B:315:VAL:HG11	2:B:346:ILE:HG12	2.03	0.41
2:B:327:GLY:O	2:B:330:SER:HB2	2.20	0.41
2:B:413:GLN:HA	2:B:414:LYS:HE2	2.02	0.41
1:A:62:ASN:OD1	1:A:62:ASN:O	2.39	0.41
2:B:386:VAL:C	2:B:388:ARG:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:OD1	1:A:152:ASP:HA	2.21	0.41
1:A:213:GLU:CG	1:A:215:GLN:NE2	2.69	0.41
2:B:284:ASN:OD1	2:B:366:GLY:HA3	2.21	0.41
2:B:304:VAL:O	2:B:348:ILE:N	2.53	0.41
2:B:414:LYS:N	2:B:414:LYS:HD3	2.36	0.41
1:A:177:LEU:O	1:A:185:SER:CB	2.69	0.40
2:B:247:LYS:HB3	2:B:248:PRO:HD2	2.03	0.40
2:B:260:ASN:ND2	2:B:416:SER:OG	2.54	0.40
2:B:260:ASN:HB3	2:B:263:GLY:O	2.21	0.40
2:B:331:MET:HE3	2:B:332:GLN:N	2.37	0.40
1:A:123:ASN:HB2	1:A:124:PRO:HD2	2.03	0.40
1:A:110:VAL:CG2	1:A:140:ILE:CD1	2.99	0.40
1:A:157:LEU:HD12	1:A:158:ARG:H	1.82	0.40
1:A:167:ARG:HH11	1:A:167:ARG:CB	2.35	0.40
1:A:168:ARG:O	1:A:171:THR:HB	2.21	0.40
2:B:247:LYS:C	2:B:249:PHE:N	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:OH	2:B:379:LEU:O[2_665]	2.18	0.02

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%)	142 (79%)	22 (12%)	15 (8%)	0	0
2	B	182/184 (99%)	136 (75%)	30 (16%)	16 (9%)	0	0
All	All	361/365 (99%)	278 (77%)	52 (14%)	31 (9%)	0	0

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	143	GLY
1	A	152	ASP
1	A	153	ASN
1	A	209	THR
2	B	245	GLN
2	B	246	ASP
2	B	247	LYS
2	B	260	ASN
2	B	321	GLU
2	B	351	SER
2	B	416	SER
1	A	46	ASN
1	A	48	PRO
1	A	84	ARG
1	A	167	ARG
1	A	217	GLY
2	B	400	PRO
2	B	409	LEU
1	A	169	PRO
1	A	216	GLU
2	B	262	TYR
2	B	342	GLU
2	B	296	PRO
2	B	328	LEU
2	B	373	ASN
1	A	223	PRO
2	B	423	PRO
1	A	124	PRO
1	A	184	PRO
2	B	349	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/167 (100%)	103 (62%)	64 (38%)	0	0
2	B	161/161 (100%)	98 (61%)	63 (39%)	0	0
All	All	328/328 (100%)	201 (61%)	127 (39%)	0	0

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	46	ASN
1	A	47	ASN
1	A	49	TYR
1	A	52	ARG
1	A	55	LYS
1	A	56	PHE
1	A	57	LEU
1	A	64	HIS
1	A	68	ARG
1	A	76	ASP
1	A	78	GLU
1	A	79	LYS
1	A	81	GLU
1	A	83	LEU
1	A	84	ARG
1	A	87	ARG
1	A	88	VAL
1	A	89	LEU
1	A	92	CYS
1	A	98	LEU
1	A	99	LEU
1	A	100	LEU
1	A	108	LEU
1	A	111	LEU
1	A	112	VAL
1	A	113	LEU
1	A	116	GLN
1	A	118	ILE
1	A	119	LEU
1	A	122	VAL
1	A	127	ARG
1	A	131	LYS
1	A	132	LEU
1	A	134	GLN

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Mol	Chain	Res	Type
1	A	138	ILE
1	A	139	LYS
1	A	144	THR
1	A	148	LEU
1	A	156	ASN
1	A	157	LEU
1	A	158	ARG
1	A	159	ILE
1	A	161	LYS
1	A	167	ARG
1	A	168	ARG
1	A	171	THR
1	A	172	VAL
1	A	175	PHE
1	A	177	LEU
1	A	178	SER
1	A	179	SER
1	A	181	LYS
1	A	182	ARG
1	A	183	LEU
1	A	192	LYS
1	A	206	ILE
1	A	207	GLU
1	A	211	LEU
1	A	212	GLN
1	A	213	GLU
1	A	214	GLU
1	A	218	VAL
1	A	222	MET
2	B	242	LEU
2	B	245	GLN
2	B	246	ASP
2	B	247	LYS
2	B	252	ARG
2	B	261	ASN
2	B	264	LYS
2	B	267	GLU
2	B	274	SER
2	B	279	LEU
2	B	282	LEU
2	B	283	LEU
2	B	286	LEU

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Mol	Chain	Res	Type
2	B	287	GLN
2	B	288	MET
2	B	293	LEU
2	B	295	VAL
2	B	304	VAL
2	B	306	LEU
2	B	312	ARG
2	B	315	VAL
2	B	317	LEU
2	B	318	VAL
2	B	320	LEU
2	B	322	GLN
2	B	323	GLN
2	B	324	GLN
2	B	325	GLN
2	B	328	LEU
2	B	329	GLU
2	B	330	SER
2	B	331	MET
2	B	332	GLN
2	B	339	THR
2	B	341	SER
2	B	344	ASP
2	B	345	ILE
2	B	346	ILE
2	B	347	VAL
2	B	354	VAL
2	B	357	LYS
2	B	362	LEU
2	B	373	ASN
2	B	375	GLU
2	B	376	ARG
2	B	383	LYS
2	B	386	VAL
2	B	387	ILE
2	B	388	ARG
2	B	389	GLN
2	B	392	ARG
2	B	394	VAL
2	B	396	ASP
2	B	404	GLU
2	B	409	LEU

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Mol	Chain	Res	Type
2	B	410	LEU
2	B	411	GLU
2	B	414	LYS
2	B	415	GLU
2	B	418	PHE
2	B	419	VAL
2	B	422	GLN
2	B	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	103	HIS
1	A	123	ASN
1	A	134	GLN
1	A	156	ASN
1	A	215	GLN
2	B	261	ASN
2	B	289	ASN
2	B	309	ASN
2	B	370	ASN
2	B	377	ASN
2	B	389	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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 [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	A	181/181 (100%)	-0.91	0 100 100	7, 19, 32, 37	0
2	B	184/184 (100%)	-0.82	1 (0%) 87 85	5, 20, 34, 45	0
All	All	365/365 (100%)	-0.87	1 (0%) 90 88	5, 19, 34, 45	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	327	GLY	2.8

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.