Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 04:25 PM EST

PDB ID	:	1CAV
Title	:	THE THREE-DIMENSIONAL STRUCTURE OF CANAVALIN FROM JACK BEAN (CANAVALIA 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:

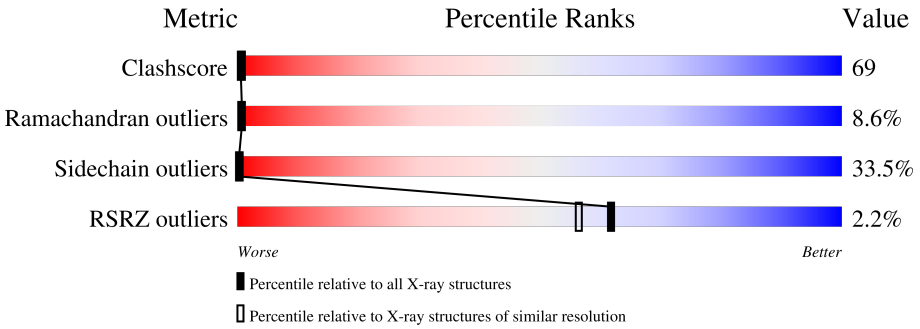
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	2% 21% 40% 31% 8%
2	B	184	2% 18% 43% 31% 8%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	181	1480	946	251	281	2	0	0	0

- Molecule 2 is a protein called CANAVALIN.

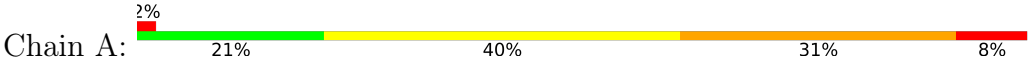
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	184	1450	902	255	289	4	0	0	0

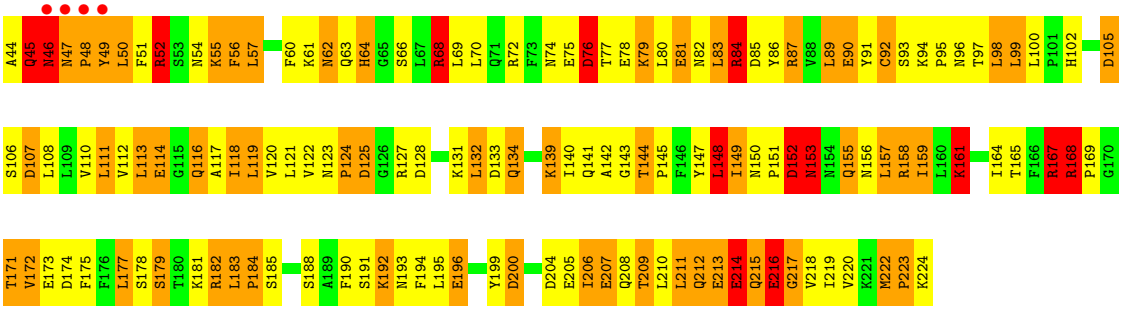
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CANAVALIN

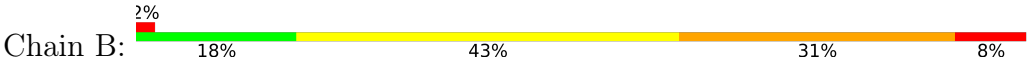
Chain A:

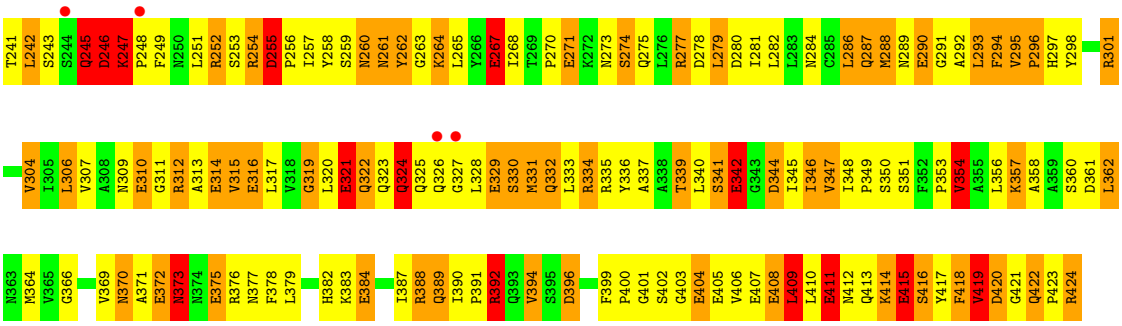




• Molecule 2: CANAVALIN

Chain B:





4 Data and refinement statistics (i)

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 36.47 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 65.4 (36.47-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.30 , 122.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	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 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	1.25	11/1511 (0.7%)	1.61	38/2046 (1.9%)
2	B	1.39	18/1472 (1.2%)	1.67	34/1992 (1.7%)
All	All	1.32	29/2983 (1.0%)	1.64	72/4038 (1.8%)

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 (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	290	GLU	CD-OE1	8.51	1.35	1.25
2	B	310	GLU	CD-OE1	8.35	1.34	1.25
2	B	375	GLU	CD-OE2	8.01	1.34	1.25
1	A	196	GLU	CD-OE1	7.86	1.34	1.25
2	B	407	GLU	CD-OE2	7.66	1.34	1.25
1	A	81	GLU	CD-OE1	7.29	1.33	1.25
1	A	216	GLU	CD-OE1	7.25	1.33	1.25
2	B	404	GLU	CD-OE1	7.11	1.33	1.25
2	B	267	GLU	CD-OE1	7.09	1.33	1.25
2	B	411	GLU	CD-OE1	7.02	1.33	1.25
2	B	314	GLU	CD-OE2	7.01	1.33	1.25
1	A	75	GLU	CD-OE2	6.90	1.33	1.25
1	A	213	GLU	CD-OE1	6.78	1.33	1.25
1	A	214	GLU	CD-OE2	6.64	1.32	1.25
2	B	316	GLU	CD-OE2	6.63	1.32	1.25
2	B	342	GLU	CD-OE1	6.58	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	415	GLU	CD-OE1	6.50	1.32	1.25
2	B	321	GLU	CD-OE2	6.41	1.32	1.25
1	A	90	GLU	CD-OE1	6.32	1.32	1.25
2	B	408	GLU	CD-OE1	6.27	1.32	1.25
1	A	52	ARG	NE-CZ	6.04	1.41	1.33
2	B	384	GLU	CD-OE2	5.71	1.31	1.25
1	A	205	GLU	CD-OE1	5.65	1.31	1.25
1	A	114	GLU	CD-OE1	5.62	1.31	1.25
2	B	372	GLU	CD-OE2	5.50	1.31	1.25
2	B	271	GLU	CD-OE2	5.33	1.31	1.25
1	A	78	GLU	CD-OE2	5.27	1.31	1.25
2	B	319	GLY	CA-C	5.11	1.60	1.51
2	B	253	SER	N-CA	5.00	1.56	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	247	LYS	C-N-CD	-13.57	90.75	120.60
2	B	420	ASP	CB-CG-OD2	8.69	126.12	118.30
1	A	105	ASP	CB-CG-OD1	-8.55	110.60	118.30
2	B	280	ASP	CB-CG-OD1	-8.38	110.76	118.30
2	B	420	ASP	CB-CG-OD1	-8.27	110.86	118.30
2	B	280	ASP	CB-CG-OD2	8.26	125.74	118.30
2	B	246	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	128	ASP	CB-CG-OD1	-7.71	111.36	118.30
2	B	255	ASP	CB-CG-OD2	-7.60	111.46	118.30
2	B	301	ARG	NE-CZ-NH1	7.29	123.95	120.30
2	B	392	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	68	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	128	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	214	GLU	N-CA-C	-6.92	92.30	111.00
1	A	168	ARG	C-N-CD	-6.92	105.37	120.60
2	B	246	ASP	CB-CG-OD1	6.83	124.45	118.30
2	B	255	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	46	ASN	N-CA-C	6.80	129.35	111.00
2	B	246	ASP	N-CA-C	6.78	129.31	111.00
1	A	152	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	105	ASP	CB-CG-OD2	6.72	124.35	118.30
2	B	344	ASP	CB-CG-OD1	-6.70	112.27	118.30
1	A	85	ASP	CB-CG-OD2	-6.67	112.30	118.30
2	B	419	VAL	N-CA-CB	-6.44	97.34	111.50
1	A	161	LYS	N-CA-CB	6.43	122.18	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	A	153	ASN	CA-C-N	-6.27	103.41	117.20
1	A	215	GLN	CB-CA-C	6.24	122.87	110.40
1	A	125	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	149	ILE	CB-CA-C	-6.20	99.20	111.60
2	B	420	ASP	N-CA-CB	6.19	121.74	110.60
1	A	153	ASN	C-N-CA	6.16	137.09	121.70
2	B	376	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	174	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	155	GLN	N-CA-CB	6.11	121.59	110.60
2	B	252	ARG	NE-CZ-NH1	6.09	123.35	120.30
2	B	278	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	204	ASP	CB-CG-OD2	6.03	123.73	118.30
2	B	324	GLN	N-CA-C	-6.00	94.80	111.00
2	B	278	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	107	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	B	392	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	174	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	107	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	50	LEU	N-CA-CB	5.72	121.85	110.40
2	B	396	ASP	CB-CG-OD1	-5.65	113.22	118.30
2	B	254	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	133	ASP	CB-CG-OD2	-5.63	113.23	118.30
2	B	373	ASN	N-CA-C	5.63	126.19	111.00
1	A	200	ASP	CB-CG-OD1	-5.58	113.27	118.30
1	A	204	ASP	CB-CG-OD1	-5.58	113.27	118.30
1	A	216	GLU	N-CA-C	-5.56	95.98	111.00
2	B	294	PHE	N-CA-C	-5.55	96.02	111.00
1	A	133	ASP	CB-CG-OD1	5.53	123.28	118.30
2	B	321	GLU	N-CA-C	5.53	125.93	111.00
1	A	148	LEU	CB-CA-C	5.47	120.60	110.20
1	A	50	LEU	CB-CA-C	5.47	120.60	110.20
1	A	153	ASN	N-CA-C	5.45	125.70	111.00
1	A	125	ASP	CB-CG-OD2	5.40	123.16	118.30
2	B	306	LEU	N-CA-CB	5.37	121.14	110.40
1	A	216	GLU	C-N-CA	5.35	133.54	122.30
2	B	301	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	72	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	B	334	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	B	354	VAL	CB-CA-C	-5.26	101.40	111.40
2	B	361	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	76	ASP	CB-CG-OD2	5.15	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	GLU	N-CA-CB	5.15	119.88	110.60
2	B	245	GLN	C-N-CA	5.09	134.42	121.70
2	B	350	SER	N-CA-C	5.06	124.65	111.00
1	A	183	LEU	C-N-CD	-5.05	109.48	120.60
2	B	319	GLY	C-N-CA	5.04	134.30	121.70

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1480	0	1473	229	1
2	B	1450	0	1425	190	1
All	All	2930	0	2898	404	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 69.

All (404) 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
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
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
2:B:331:MET:HE2	2:B:332:GLN:H	1.40	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
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
2:B:329:GLU:CD	2:B:329:GLU:H	1.82	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:213:GLU:HG2	1:A:215:GLN:NE2	2.05	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
2:B:288:MET:HE2	2:B:358:ALA:HB2	1.72	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
2:B:247:LYS:C	2:B:249:PHE:H	1.96	0.68
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
2:B:316:GLU:CG	2:B:335:ARG:HD2	2.24	0.68
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
2:B:412:ASN:C	2:B:414:LYS:HE2	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:286:LEU:C	2:B:286:LEU:HD22	2.18	0.63
1:A:179:SER:OG	1:A:211:LEU:HA	1.99	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:411:GLU:C	2:B:413:GLN:H	1.99	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:260:ASN:CG	2:B:261:ASN:H	1.97	0.62
2:B:307:VAL:HG22	2:B:345:ILE:CG1	2.29	0.62
1:A:62:ASN:OD1	1:A:62:ASN:C	2.37	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
1:A:212:GLN:CD	1:A:213:GLU:N	2.53	0.61
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
2:B:331:MET:CE	2:B:332:GLN:N	2.63	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:331:MET:HE2	2:B:332:GLN:HB2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:GLU:HG3	2:B:335:ARG:HD2	1.82	0.60
2:B:243:SER:C	2:B:245:GLN:H	2.04	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: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:111:LEU:C	1:A:111:LEU:HD12	2.22	0.59
2:B:324:GLN:O	2:B:324:GLN:HG3	2.02	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:56:PHE:HB3	1:A:69:LEU:C	2.23	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:48:PRO:O	1:A:77:THR:HA	2.05	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
1:A:76:ASP:OD1	1:A:76:ASP:N	2.38	0.56
2:B:297:HIS:O	2:B:353:PRO:HA	2.04	0.56
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: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
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:262:TYR:HH	2:B:420:ASP:HB2	1.71	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:282:LEU:C	2:B:282:LEU:HD12	2.27	0.55
1:A:157:LEU:HD12	1:A:157:LEU:C	2.24	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: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
1:A:151:PRO:C	1:A:153:ASN:H	2.11	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
2:B:331:MET:HE3	2:B:332:GLN:N	2.23	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
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: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
1:A:79:LYS:HZ1	2:B:321:GLU:C	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:172:VAL:C	1:A:173:GLU:HG2	2.31	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
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
2:B:371:ALA:O	2:B:372:GLU:C	2.49	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
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
1:A:212:GLN:CD	1:A:213:GLU:C	2.70	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
2:B:373:ASN:ND2	2:B:373:ASN:O	2.45	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
2:B:288:MET:HE3	2:B:292:ALA:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:288:MET:HE2	2:B:358:ALA:CB	2.41	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
2:B:411:GLU:C	2:B:413:GLN:N	2.67	0.48
1:A:206:ILE:HG23	1:A:210:LEU:HD13	1.96	0.48
1:A:57:LEU:N	1:A:57:LEU:HD22	2.28	0.47
1:A:118:ILE:HD13	1:A:151:PRO:HG3	1.96	0.47
1:A:118:ILE:N	1:A:118:ILE:CD1	2.76	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:HD13	1:A:118:ILE:N	2.30	0.47
1:A:219:ILE:C	1:A:220:VAL:HG23	2.34	0.47
2:B:273:ASN:O	2:B:277:ARG:HB2	2.15	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
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
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
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:292:ALA:O	2:B:293:LEU:C	2.53	0.46
2:B:408:GLU:C	2:B:410:LEU:N	2.68	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
2:B:331:MET:HE1	2:B:332:GLN:HB2	1.96	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:192:LYS:CG	1:A:193:ASN:N	2.78	0.46
1:A:167:ARG:NH1	1:A:167:ARG:CB	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:98:LEU:HD23	1:A:149:ILE:HG12	1.98	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
2:B:408:GLU:O	2:B:409:LEU:C	2.53	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
2:B:325:GLN:CD	2:B:331:MET:HG2	2.36	0.45
2:B:288:MET:CE	2:B:292:ALA:O	2.65	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:413:GLN:O	2:B:413:GLN:HG3	2.17	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
2:B:262:TYR:CE1	2:B:420:ASP:CA	2.98	0.45
2:B:295:VAL:O	2:B:296:PRO:C	2.56	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
1:A:219:ILE:C	1:A:220:VAL:CG2	2.85	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:241:THR:HG23	2:B:249:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:419:VAL:CG1	2:B:420:ASP:N	2.80	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
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: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
1:A:212:GLN:CD	1:A:214:GLU:N	2.72	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
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
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
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
1:A:215:GLN:O	1:A:216:GLU:C	2.56	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
2:B:288:MET:HE2	2:B:288:MET:HB2	1.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:HB3	1:A:79:LYS:HD3	1.97	0.42
2:B:341:SER:O	2:B:342:GLU:C	2.58	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:119:LEU:C	1:A:119:LEU:HD23	2.40	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: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
1:A:96:ASN:OD1	1:A:152:ASP:HA	2.21	0.41
1:A:117:ALA:C	1:A:118:ILE:HD13	2.41	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:289:ASN:O	2:B:290:GLU:C	2.59	0.41
2:B:304:VAL:O	2:B:348:ILE:N	2.53	0.41
1:A:212:GLN:NE2	1:A:213:GLU:C	2.74	0.41
2:B:414:LYS:N	2:B:414:LYS:HD3	2.36	0.41
1:A:117:ALA:C	1:A:118:ILE:CD1	2.90	0.40
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
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

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 (i)

5.3.1 Protein backbone (i)

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%)	1	1
2	B	182/184 (99%)	136 (75%)	30 (16%)	16 (9%)	1	0
All	All	361/365 (99%)	278 (77%)	52 (14%)	31 (9%)	1	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

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Mol	Chain	Res	Type
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 (i)

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%)	111 (66%)	56 (34%)	0	0
2	B	161/161 (100%)	107 (66%)	54 (34%)	0	0
All	All	328/328 (100%)	218 (66%)	110 (34%)	0	0

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
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	61	LYS
1	A	64	HIS
1	A	68	ARG
1	A	76	ASP
1	A	79	LYS
1	A	81	GLU
1	A	83	LEU
1	A	84	ARG
1	A	87	ARG
1	A	89	LEU

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Mol	Chain	Res	Type
1	A	92	CYS
1	A	98	LEU
1	A	99	LEU
1	A	108	LEU
1	A	111	LEU
1	A	113	LEU
1	A	116	GLN
1	A	118	ILE
1	A	119	LEU
1	A	127	ARG
1	A	132	LEU
1	A	134	GLN
1	A	139	LYS
1	A	144	THR
1	A	148	LEU
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	188	SER
1	A	192	LYS
1	A	200	ASP
1	A	206	ILE
1	A	207	GLU
1	A	211	LEU
1	A	212	GLN
1	A	214	GLU
1	A	222	MET
2	B	242	LEU
2	B	245	GLN
2	B	246	ASP

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Mol	Chain	Res	Type
2	B	247	LYS
2	B	252	ARG
2	B	255	ASP
2	B	261	ASN
2	B	264	LYS
2	B	267	GLU
2	B	274	SER
2	B	277	ARG
2	B	279	LEU
2	B	286	LEU
2	B	287	GLN
2	B	288	MET
2	B	293	LEU
2	B	294	PHE
2	B	295	VAL
2	B	304	VAL
2	B	312	ARG
2	B	315	VAL
2	B	317	LEU
2	B	322	GLN
2	B	324	GLN
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	346	ILE
2	B	347	VAL
2	B	354	VAL
2	B	357	LYS
2	B	362	LEU
2	B	370	ASN
2	B	373	ASN
2	B	375	GLU
2	B	383	LYS
2	B	388	ARG
2	B	389	GLN
2	B	392	ARG
2	B	394	VAL
2	B	396	ASP

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Mol	Chain	Res	Type
2	B	404	GLU
2	B	409	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 (11) 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	141	GLN
1	A	156	ASN
1	A	215	GLN
2	B	261	ASN
2	B	309	ASN
2	B	370	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 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, 95^{th} 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%)	-0.85	4 (2%)	62	56	7, 19, 32, 37	0
2	B	184/184 (100%)	-0.65	4 (2%)	62	56	5, 20, 34, 45	0
All	All	365/365 (100%)	-0.75	8 (2%)	62	56	5, 19, 34, 45	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	PRO	4.9
1	A	49	TYR	4.6
2	B	327	GLY	2.9
1	A	46	ASN	2.8
2	B	244	SER	2.7
2	B	326	GLN	2.4
1	A	47	ASN	2.4
2	B	248	PRO	2.2

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 (i)

There are no such residues in this entry.