



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:57 AM UTC

PDB ID : 1CAW / pdb_00001caw
Title : DETERMINATION OF THREE CRYSTAL STRUCTURES OF
CANAVALLIN BY MOLECULAR REPLACEMENT
Authors : Ko, T-P.; Ng, J.D.; Day, J.; Greenwood, A.; McPherson, A.
Deposited on : 1993-06-02
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

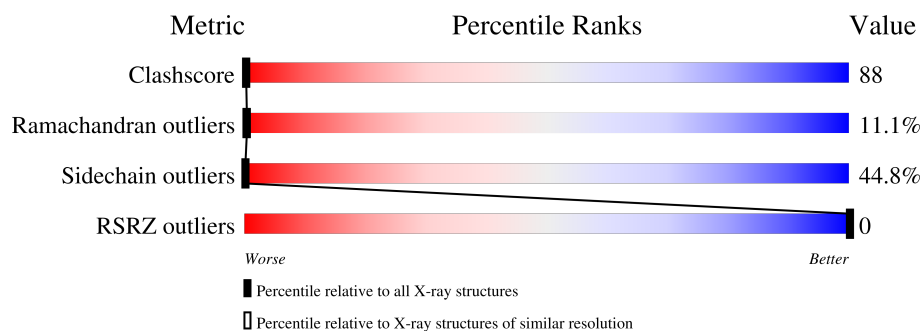
1 Overall quality at a glance

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	
2	B	184	

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			

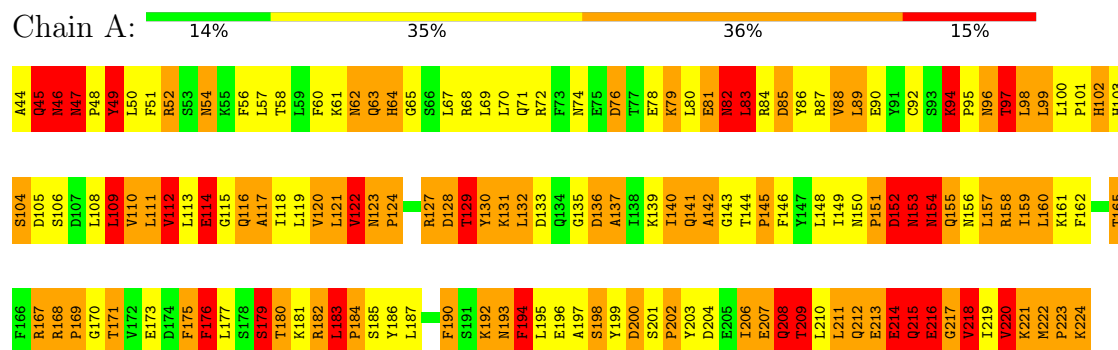
- Molecule 2 is a protein called CANAVALIN.

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

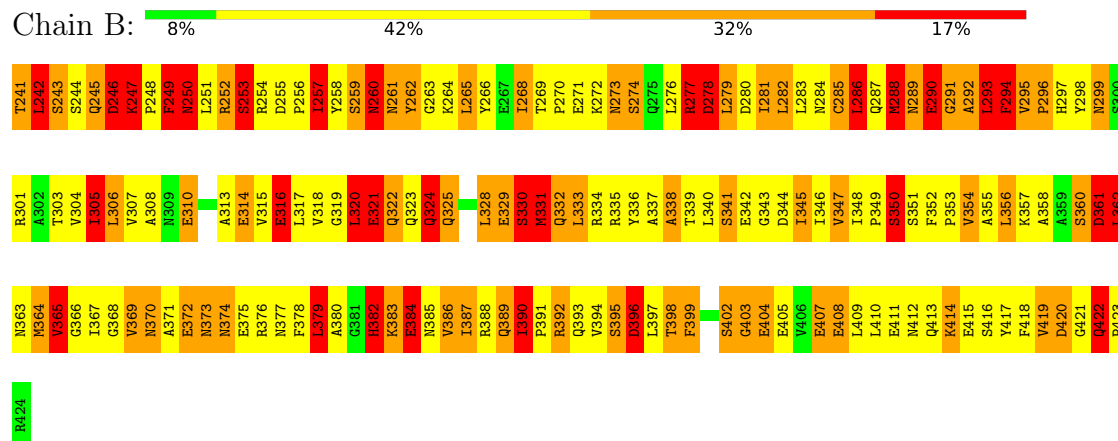
3 Residue-property plots

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	H 3	Depositor
Cell constants a, b, c, α , β , γ	136.80Å 136.80Å 75.70Å 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) 64.6 (8.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.57Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.194 , (Not available) 0.204 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.436 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2930	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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	1.61	14/1511 (0.9%)	2.07	63/2046 (3.1%)
2	B	1.63	13/1472 (0.9%)	2.11	56/1992 (2.8%)
All	All	1.62	27/2983 (0.9%)	2.09	119/4038 (2.9%)

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	1	1
2	B	1	1
All	All	2	2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	285	CYS	C-N	-7.87	1.23	1.33
2	B	383	LYS	N-CA	-7.38	1.37	1.45
2	B	383	LYS	CA-C	-7.26	1.43	1.52
2	B	252	ARG	NE-CZ	7.09	1.40	1.33
1	A	115	GLY	N-CA	6.45	1.51	1.45
1	A	216	GLU	CD-OE2	6.39	1.37	1.25
1	A	52	ARG	NE-CZ	6.37	1.40	1.33
2	B	294	PHE	C-O	-6.34	1.16	1.24
1	A	145	PRO	N-CA	-6.24	1.39	1.47
2	B	356	LEU	CA-C	-6.12	1.45	1.52
2	B	286	LEU	N-CA	-5.88	1.38	1.45
1	A	92	CYS	CA-C	-5.78	1.45	1.52
1	A	115	GLY	CA-C	5.76	1.57	1.51
1	A	160	LEU	CA-C	-5.69	1.45	1.52
2	B	338	ALA	N-CA	-5.66	1.39	1.46
1	A	145	PRO	CA-C	-5.64	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	SER	C-N	-5.49	1.26	1.33
2	B	294	PHE	CA-C	-5.46	1.46	1.52
1	A	152	ASP	N-CA	-5.45	1.39	1.46
1	A	114	GLU	C-N	5.42	1.39	1.32
1	A	197	ALA	N-CA	-5.38	1.40	1.46
1	A	132	LEU	C-N	5.36	1.40	1.33
1	A	137	ALA	N-CA	-5.22	1.39	1.46
2	B	365	VAL	CA-C	-5.18	1.46	1.52
2	B	331	MET	CA-C	-5.14	1.46	1.52
2	B	411	GLU	CD-OE1	5.12	1.35	1.25
1	A	65	GLY	CA-C	5.02	1.57	1.51

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ILE	N-CA-CB	-13.61	99.04	112.65
2	B	399	PHE	CA-CB-CG	13.07	126.87	113.80
2	B	382	HIS	CA-CB-CG	-11.42	102.38	113.80
1	A	167	ARG	N-CA-CB	11.28	126.42	110.07
2	B	324	GLN	N-CA-C	-10.57	98.18	112.03
1	A	140	ILE	CB-CA-C	9.89	121.22	111.23
2	B	247	LYS	C-N-CD	-9.87	84.54	125.00
2	B	390	ILE	N-CA-CB	9.65	123.24	111.08
2	B	332	GLN	N-CA-C	8.91	123.92	109.85
2	B	379	LEU	N-CA-CB	8.78	124.24	110.46
1	A	82	ASN	CA-CB-CG	8.70	121.30	112.60
2	B	257	ILE	N-CA-C	-8.64	99.86	111.44
2	B	408	GLU	N-CA-C	8.64	120.38	110.97
1	A	175	PHE	CA-CB-CG	8.25	122.05	113.80
1	A	153	ASN	N-CA-CB	8.20	124.34	110.49
2	B	396	ASP	CB-CA-C	-8.01	98.18	110.92
1	A	101	PRO	N-CA-CB	7.98	110.38	103.36
1	A	101	PRO	N-CA-C	7.95	122.80	110.80
2	B	286	LEU	N-CA-CB	-7.94	99.02	111.56
2	B	384	GLU	CB-CA-C	7.89	124.22	111.36
1	A	154	ASN	N-CA-C	7.87	127.57	110.80
2	B	247	LYS	CA-C-N	7.80	129.60	119.84
2	B	247	LYS	C-N-CA	7.80	129.60	119.84
1	A	179	SER	N-CA-C	7.59	121.80	109.59
2	B	242	LEU	N-CA-C	7.49	119.09	108.00
2	B	288	MET	N-CA-C	7.47	122.50	107.41
1	A	220	VAL	N-CA-C	7.47	120.35	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	GLY	N-CA-C	7.43	120.66	110.56
1	A	155	GLN	N-CA-C	7.38	120.32	109.69
1	A	96	ASN	CA-CB-CG	-7.29	105.31	112.60
2	B	292	ALA	N-CA-C	7.28	119.36	110.41
2	B	383	LYS	O-C-N	7.24	131.21	123.03
2	B	250	ASN	N-CA-C	7.18	118.65	108.74
2	B	320	LEU	N-CA-C	-7.16	97.54	109.07
2	B	371	ALA	N-CA-C	7.15	120.29	108.49
2	B	370	ASN	CA-C-N	-7.00	113.66	123.03
2	B	370	ASN	C-N-CA	-7.00	113.66	123.03
1	A	183	LEU	CA-C-N	6.85	128.41	119.84
1	A	183	LEU	C-N-CA	6.85	128.41	119.84
1	A	78	GLU	N-CA-C	-6.79	104.61	113.17
1	A	198	SER	N-CA-C	6.73	119.62	111.82
1	A	218	VAL	N-CA-CB	6.65	122.21	111.23
1	A	49	TYR	CB-CA-C	6.64	122.38	111.50
1	A	109	LEU	CA-C-N	-6.63	114.45	123.14
1	A	109	LEU	C-N-CA	-6.63	114.45	123.14
2	B	323	GLN	CA-C-N	6.63	131.96	121.08
2	B	323	GLN	C-N-CA	6.63	131.96	121.08
2	B	422	GLN	CA-C-N	6.45	127.90	119.84
2	B	422	GLN	C-N-CA	6.45	127.90	119.84
2	B	293	LEU	CB-CA-C	6.43	120.91	109.65
1	A	62	ASN	CA-CB-CG	6.34	118.94	112.60
1	A	145	PRO	N-CA-C	-6.32	99.46	112.47
1	A	190	PHE	N-CA-CB	6.31	119.08	110.38
1	A	122	VAL	N-CA-C	6.25	117.12	108.12
2	B	278	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	165	THR	N-CA-C	6.20	120.17	110.32
1	A	154	ASN	CA-CB-CG	-6.13	106.47	112.60
2	B	322	GLN	N-CA-CB	6.10	120.80	110.49
2	B	246	ASP	N-CA-CB	6.04	120.70	110.49
2	B	268	ILE	N-CA-CB	6.01	118.20	110.99
1	A	151	PRO	N-CA-CB	5.95	109.50	103.25
1	A	82	ASN	N-CA-CB	5.92	120.50	110.49
1	A	129	THR	N-CA-C	5.82	119.87	107.70
1	A	211	LEU	N-CA-C	5.79	119.34	107.69
2	B	260	ASN	CA-CB-CG	5.79	118.39	112.60
2	B	273	ASN	CA-CB-CG	-5.75	106.84	112.60
1	A	190	PHE	CA-CB-CG	5.75	119.55	113.80
2	B	280	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	217	GLY	N-CA-C	5.73	126.76	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	398	THR	N-CA-C	5.70	120.23	113.28
2	B	320	LEU	CA-C-N	-5.64	110.77	121.54
2	B	320	LEU	C-N-CA	-5.64	110.77	121.54
1	A	169	PRO	N-CA-CB	5.63	109.17	103.25
1	A	117	ALA	N-CA-C	5.63	118.42	110.14
2	B	361	ASP	N-CA-C	-5.57	98.94	110.80
1	A	122	VAL	CB-CA-C	5.55	118.43	110.33
1	A	110	VAL	CB-CA-C	5.54	118.83	110.63
1	A	194	PHE	CB-CA-C	5.54	121.20	110.46
1	A	117	ALA	CA-C-N	5.51	131.11	122.84
1	A	117	ALA	C-N-CA	5.51	131.11	122.84
1	A	47	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	97	THR	N-CA-CB	-5.49	101.69	111.08
1	A	49	TYR	CA-CB-CG	5.48	123.76	113.90
1	A	179	SER	CB-CA-C	5.47	119.23	109.38
1	A	127	ARG	N-CA-C	-5.46	101.23	109.85
1	A	49	TYR	CA-C-N	-5.37	113.22	123.32
1	A	49	TYR	C-N-CA	-5.37	113.22	123.32
1	A	140	ILE	CA-CB-CG1	5.37	119.52	110.40
2	B	362	LEU	N-CA-C	5.33	117.43	108.96
1	A	94	LYS	CA-C-N	5.33	126.50	119.84
1	A	94	LYS	C-N-CA	5.33	126.50	119.84
1	A	176	PHE	CA-C-N	5.32	127.72	120.54
1	A	176	PHE	C-N-CA	5.32	127.72	120.54
2	B	321	GLU	N-CA-C	5.32	122.13	110.80
1	A	218	VAL	N-CA-C	-5.28	98.35	109.34
1	A	110	VAL	N-CA-C	5.28	115.50	108.11
2	B	255	ASP	N-CA-C	5.26	117.71	108.82
2	B	389	GLN	CB-CA-C	5.20	119.36	110.01
1	A	152	ASP	CB-CA-C	5.19	120.75	110.42
2	B	249	PHE	N-CA-C	5.18	121.84	110.80
2	B	422	GLN	N-CA-CB	5.16	119.56	110.37
2	B	294	PHE	CA-CB-CG	-5.15	108.65	113.80
2	B	305	ILE	N-CA-C	-5.15	101.03	108.71
2	B	373	ASN	N-CA-C	5.13	118.20	111.28
2	B	403	GLY	O-C-N	5.12	127.20	122.13
1	A	112	VAL	N-CA-CB	5.11	117.48	111.66
2	B	390	ILE	CA-CB-CG1	5.08	119.03	110.40
2	B	422	GLN	O-C-N	5.07	127.15	121.32
1	A	45	GLN	CA-C-N	5.07	131.22	121.54
1	A	45	GLN	C-N-CA	5.07	131.22	121.54
2	B	316	GLU	CB-CA-C	5.07	118.50	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	253	SER	N-CA-C	5.05	116.87	107.99
1	A	116	GLN	CA-C-N	-5.04	114.04	123.05
1	A	116	GLN	C-N-CA	-5.04	114.04	123.05
1	A	128	ASP	CA-C-N	-5.04	115.70	122.95
1	A	128	ASP	C-N-CA	-5.04	115.70	122.95
2	B	390	ILE	CA-C-N	5.00	124.93	119.78
2	B	390	ILE	C-N-CA	5.00	124.93	119.78
2	B	420	ASP	CA-CB-CG	5.00	117.60	112.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	153	ASN	CA
2	B	379	LEU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	GLU	Mainchain
2	B	396	ASP	Sidechain

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	278	0
2	B	1450	0	1425	257	0
All	All	2930	0	2898	514	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 88.

All (514) 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:286:LEU:HD13	2:B:287:GLN:N	1.53	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:HD13	2:B:286:LEU:C	1.69	1.17
2:B:265:LEU:HD12	2:B:286:LEU:HB2	1.17	1.11
1:A:120:VAL:HG13	1:A:129:THR:HG23	1.33	1.09
1:A:108:LEU:HB2	1:A:140:ILE:HG23	1.31	1.07
1:A:131:LYS:HE2	2:B:241:THR:HG23	1.36	1.05
2:B:257:ILE:HD11	2:B:265:LEU:HD23	1.41	1.03
1:A:113:LEU:HD11	1:A:160:LEU:HB2	1.41	0.99
2:B:251:LEU:HD13	2:B:268:ILE:HD13	1.44	0.98
2:B:286:LEU:C	2:B:286:LEU:CD1	2.37	0.97
2:B:250:ASN:HD22	2:B:251:LEU:H	1.04	0.96
1:A:114:GLU:HG2	1:A:158:ARG:HH11	1.31	0.96
1:A:179:SER:HB3	1:A:184:PRO:HA	1.50	0.91
1:A:58:THR:HG21	1:A:61:LYS:HE3	1.49	0.90
1:A:56:PHE:CE1	1:A:70:LEU:HD13	2.05	0.90
1:A:123:ASN:HB2	1:A:124:PRO:HD2	1.53	0.89
2:B:276:LEU:HD21	2:B:283:LEU:HD23	1.53	0.89
2:B:322:GLN:HE21	2:B:324:GLN:HB2	1.37	0.89
2:B:315:VAL:HG11	2:B:346:ILE:CD1	2.04	0.88
2:B:265:LEU:CD1	2:B:286:LEU:HB2	2.03	0.87
2:B:340:LEU:HB3	2:B:344:ASP:HB2	1.57	0.87
1:A:49:TYR:CE1	1:A:79:LYS:HD2	2.10	0.86
1:A:72:ARG:NH1	1:A:171:THR:N	2.24	0.86
2:B:257:ILE:HD11	2:B:265:LEU:CD2	2.06	0.86
1:A:193:ASN:HB2	1:A:194:PHE:HD1	1.39	0.86
1:A:45:GLN:OE1	1:A:46:ASN:N	2.08	0.85
1:A:111:LEU:HD23	1:A:160:LEU:HD23	1.57	0.85
1:A:114:GLU:HG2	1:A:158:ARG:NH1	1.93	0.84
1:A:113:LEU:CD1	1:A:160:LEU:HB2	2.07	0.84
2:B:260:ASN:ND2	2:B:416:SER:OG	2.10	0.84
1:A:47:ASN:CG	1:A:48:PRO:HD2	2.02	0.84
1:A:131:LYS:HE2	2:B:241:THR:CG2	2.07	0.84
1:A:222:MET:HE2	1:A:224:LYS:CG	2.07	0.84
1:A:72:ARG:HH12	1:A:171:THR:N	1.77	0.83
1:A:69:LEU:HD21	1:A:87:ARG:NH1	1.94	0.82
1:A:192:LYS:HA	1:A:203:TYR:CD1	2.14	0.82
1:A:70:LEU:CB	1:A:88:VAL:HG12	2.09	0.82
2:B:265:LEU:HD12	2:B:286:LEU:CB	2.08	0.82
2:B:335:ARG:NH1	2:B:337:ALA:HB2	1.94	0.82
2:B:261:ASN:HD22	2:B:261:ASN:C	1.88	0.81
1:A:108:LEU:CB	1:A:140:ILE:HG23	2.10	0.81
2:B:414:LYS:H	2:B:414:LYS:HD3	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:PRO:CB	2:B:277:ARG:HA	2.11	0.81
1:A:111:LEU:HB2	1:A:160:LEU:HB3	1.60	0.81
1:A:131:LYS:CE	2:B:241:THR:HG23	2.10	0.80
2:B:322:GLN:HE21	2:B:324:GLN:CB	1.94	0.80
1:A:70:LEU:HD22	2:B:345:ILE:HD13	1.64	0.80
1:A:155:GLN:HG2	1:A:156:ASN:H	1.45	0.80
2:B:270:PRO:HB3	2:B:277:ARG:N	1.97	0.80
1:A:116:GLN:O	1:A:151:PRO:HD2	1.82	0.80
2:B:262:TYR:C	2:B:289:ASN:HD22	1.89	0.80
2:B:303:THR:O	2:B:369:VAL:HG23	1.81	0.79
2:B:257:ILE:HD12	2:B:258:TYR:CE2	2.18	0.79
2:B:250:ASN:ND2	2:B:251:LEU:H	1.80	0.78
1:A:199:TYR:HB2	1:A:206:ILE:HD11	1.65	0.78
1:A:131:LYS:H	2:B:241:THR:HA	1.49	0.78
1:A:199:TYR:CB	1:A:206:ILE:HD11	2.13	0.78
1:A:60:PHE:CE2	1:A:218:VAL:HB	2.19	0.77
1:A:222:MET:HE2	1:A:224:LYS:HG3	1.65	0.77
1:A:215:GLN:O	1:A:217:GLY:N	2.17	0.77
1:A:110:VAL:HG13	1:A:159:ILE:HG23	1.64	0.77
2:B:315:VAL:N	2:B:338:ALA:O	2.16	0.77
1:A:72:ARG:HH11	1:A:170:GLY:HA3	1.50	0.76
1:A:123:ASN:HB2	1:A:124:PRO:CD	2.15	0.76
1:A:49:TYR:O	1:A:49:TYR:HD1	1.68	0.76
1:A:74:ASN:HB2	1:A:81:GLU:OE2	1.86	0.75
1:A:110:VAL:CG1	1:A:159:ILE:HD12	2.16	0.75
1:A:122:VAL:HG23	1:A:127:ARG:HA	1.68	0.75
1:A:113:LEU:HD22	2:B:365:VAL:HG21	1.68	0.75
2:B:379:LEU:HD13	2:B:379:LEU:N	2.02	0.75
1:A:87:ARG:HG2	1:A:170:GLY:O	1.86	0.75
1:A:79:LYS:O	1:A:80:LEU:HD23	1.87	0.74
2:B:315:VAL:HG11	2:B:346:ILE:HD13	1.66	0.74
2:B:269:THR:HG22	2:B:282:LEU:HD11	1.67	0.74
2:B:253:SER:HB3	2:B:266:TYR:CD2	2.23	0.74
1:A:112:VAL:HG13	1:A:159:ILE:CD1	2.18	0.73
2:B:253:SER:OG	2:B:266:TYR:HB3	1.89	0.73
1:A:108:LEU:HB2	1:A:140:ILE:CG2	2.16	0.73
2:B:270:PRO:HB3	2:B:277:ARG:HA	1.71	0.73
1:A:79:LYS:HE3	2:B:321:GLU:CD	2.13	0.72
1:A:144:THR:HG22	1:A:145:PRO:O	1.88	0.72
2:B:322:GLN:O	2:B:331:MET:HG3	1.87	0.72
2:B:279:LEU:N	2:B:279:LEU:HD23	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:HIS:HB2	1:A:143:GLY:O	1.90	0.72
2:B:268:ILE:O	2:B:282:LEU:HD12	1.89	0.72
2:B:278:ASP:C	2:B:279:LEU:HD23	2.15	0.72
2:B:340:LEU:HB3	2:B:344:ASP:CB	2.19	0.72
1:A:56:PHE:HB3	1:A:68:ARG:HB3	1.72	0.71
1:A:109:LEU:HB2	1:A:162:PHE:HB3	1.72	0.71
2:B:286:LEU:HD13	2:B:287:GLN:CA	2.20	0.71
2:B:412:ASN:O	2:B:414:LYS:HD3	1.90	0.71
1:A:63:GLN:O	1:A:64:HIS:ND1	2.24	0.71
1:A:70:LEU:HB2	1:A:88:VAL:HG12	1.72	0.70
1:A:193:ASN:HB2	1:A:194:PHE:CD1	2.23	0.70
2:B:404:GLU:O	2:B:408:GLU:HG2	1.90	0.70
2:B:392:ARG:HD2	2:B:407:GLU:OE2	1.91	0.70
2:B:249:PHE:HD1	2:B:249:PHE:H	1.36	0.70
1:A:70:LEU:HB3	1:A:88:VAL:HG12	1.73	0.70
1:A:117:ALA:O	1:A:132:LEU:N	2.25	0.70
1:A:187:LEU:O	1:A:195:LEU:HD11	1.92	0.69
1:A:97:THR:O	1:A:149:ILE:HG23	1.92	0.69
2:B:270:PRO:HB2	2:B:277:ARG:HA	1.74	0.69
1:A:62:ASN:HD22	1:A:216:GLU:HB2	1.57	0.69
1:A:199:TYR:HB2	1:A:206:ILE:CD1	2.22	0.69
2:B:313:ALA:HB2	2:B:362:LEU:CD1	2.22	0.69
2:B:289:ASN:O	2:B:291:GLY:N	2.26	0.69
2:B:265:LEU:HD12	2:B:286:LEU:HD23	1.75	0.68
1:A:58:THR:CG2	1:A:61:LYS:HB2	2.23	0.68
2:B:414:LYS:H	2:B:414:LYS:CD	2.01	0.68
2:B:261:ASN:O	2:B:289:ASN:ND2	2.27	0.68
2:B:299:ASN:O	2:B:350:SER:O	2.12	0.68
1:A:114:GLU:CG	1:A:158:ARG:HH11	2.06	0.68
2:B:310:GLU:HB3	2:B:363:ASN:H	1.57	0.68
2:B:373:ASN:ND2	2:B:373:ASN:O	2.27	0.68
2:B:416:SER:OG	2:B:417:TYR:N	2.27	0.68
2:B:262:TYR:O	2:B:289:ASN:ND2	2.27	0.67
2:B:276:LEU:O	2:B:278:ASP:N	2.28	0.67
2:B:328:LEU:HD12	2:B:329:GLU:H	1.59	0.67
2:B:256:PRO:HD3	2:B:266:TYR:CZ	2.30	0.66
1:A:97:THR:CG2	1:A:221:LYS:HZ1	2.09	0.66
1:A:109:LEU:CB	1:A:162:PHE:HB3	2.25	0.66
1:A:83:LEU:HA	1:A:86:TYR:CD2	2.30	0.66
2:B:288:MET:HE2	2:B:292:ALA:C	2.20	0.66
1:A:81:GLU:O	1:A:84:ARG:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:CD2	2:B:369:VAL:HG21	2.26	0.66
1:A:103:HIS:HA	1:A:144:THR:O	1.96	0.65
1:A:49:TYR:O	1:A:49:TYR:CD1	2.49	0.65
2:B:392:ARG:O	2:B:396:ASP:OD1	2.15	0.65
1:A:105:ASP:OD1	1:A:106:SER:N	2.29	0.65
1:A:49:TYR:OH	1:A:79:LYS:HE2	1.96	0.65
2:B:257:ILE:CD1	2:B:265:LEU:HD23	2.23	0.65
2:B:398:THR:HG22	2:B:399:PHE:CD1	2.31	0.65
1:A:113:LEU:O	1:A:114:GLU:HB3	1.97	0.65
2:B:315:VAL:HG11	2:B:346:ILE:HD11	1.79	0.65
1:A:221:LYS:C	1:A:222:MET:HG3	2.22	0.65
2:B:265:LEU:CD1	2:B:286:LEU:HD23	2.26	0.65
1:A:83:LEU:HA	1:A:86:TYR:HD2	1.61	0.64
2:B:360:SER:O	2:B:362:LEU:N	2.31	0.64
1:A:47:ASN:ND2	1:A:48:PRO:HD2	2.12	0.64
2:B:378:PHE:HD2	2:B:384:GLU:CB	2.10	0.64
1:A:221:LYS:HZ3	1:A:221:LYS:HB2	1.63	0.64
2:B:316:GLU:O	2:B:354:VAL:HG23	1.98	0.64
2:B:332:GLN:HA	2:B:332:GLN:OE1	1.97	0.64
1:A:72:ARG:HH11	1:A:170:GLY:CA	2.11	0.64
1:A:85:ASP:HA	1:A:170:GLY:CA	2.28	0.63
1:A:214:GLU:O	1:A:215:GLN:O	2.16	0.63
2:B:328:LEU:CD1	2:B:329:GLU:H	2.11	0.63
1:A:133:ASP:OD2	2:B:252:ARG:NH2	2.31	0.63
1:A:70:LEU:O	1:A:87:ARG:NH1	2.30	0.63
1:A:185:SER:OG	1:A:186:TYR:N	2.28	0.63
1:A:70:LEU:HD22	1:A:88:VAL:HG11	1.81	0.63
1:A:72:ARG:N	1:A:87:ARG:NH1	2.47	0.63
2:B:251:LEU:HD13	2:B:268:ILE:CD1	2.25	0.63
1:A:133:ASP:O	1:A:136:ASP:HB2	1.99	0.63
2:B:265:LEU:HD12	2:B:286:LEU:CD2	2.29	0.63
2:B:310:GLU:O	2:B:362:LEU:HA	1.98	0.63
1:A:208:GLN:O	1:A:209:THR:OG1	2.17	0.63
1:A:44:ALA:HB3	1:A:71:GLN:HE22	1.63	0.63
2:B:257:ILE:HD12	2:B:258:TYR:CD2	2.34	0.62
2:B:250:ASN:HD22	2:B:251:LEU:N	1.87	0.62
1:A:194:PHE:HD1	1:A:194:PHE:H	1.48	0.62
1:A:72:ARG:NH1	1:A:170:GLY:C	2.57	0.62
1:A:223:PRO:CD	1:A:224:LYS:H	2.13	0.62
1:A:213:GLU:O	1:A:214:GLU:C	2.40	0.61
1:A:213:GLU:O	1:A:213:GLU:OE1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:LEU:HD22	2:B:410:LEU:H	1.64	0.61
1:A:196:GLU:O	1:A:200:ASP:HA	2.00	0.61
2:B:313:ALA:O	2:B:339:THR:HA	2.00	0.61
1:A:221:LYS:HZ3	1:A:221:LYS:CB	2.13	0.61
2:B:269:THR:HA	2:B:282:LEU:HD13	1.83	0.61
2:B:382:HIS:HB2	2:B:415:GLU:O	2.00	0.61
1:A:123:ASN:CB	1:A:124:PRO:HD2	2.27	0.61
2:B:286:LEU:C	2:B:287:GLN:HG2	2.24	0.61
1:A:215:GLN:OE1	1:A:215:GLN:N	2.34	0.60
2:B:265:LEU:HA	2:B:286:LEU:HA	1.83	0.60
2:B:334:ARG:HG3	2:B:335:ARG:N	2.16	0.60
2:B:282:LEU:HB3	2:B:368:GLY:HA3	1.83	0.60
2:B:262:TYR:CA	2:B:289:ASN:HD22	2.13	0.60
2:B:313:ALA:HB2	2:B:362:LEU:HD11	1.82	0.60
1:A:110:VAL:O	1:A:137:ALA:HA	2.02	0.60
1:A:45:GLN:CD	1:A:46:ASN:H	2.10	0.60
1:A:194:PHE:CD1	1:A:194:PHE:N	2.70	0.60
2:B:270:PRO:HB3	2:B:277:ARG:CA	2.32	0.59
2:B:306:LEU:HG	2:B:364:MET:SD	2.42	0.59
2:B:262:TYR:HA	2:B:289:ASN:HD22	1.67	0.59
1:A:47:ASN:CB	1:A:48:PRO:HD2	2.32	0.59
1:A:112:VAL:HG13	1:A:159:ILE:HD11	1.82	0.59
1:A:135:GLY:O	1:A:136:ASP:C	2.46	0.59
1:A:150:ASN:OD1	1:A:157:LEU:HB2	2.02	0.59
1:A:182:ARG:O	1:A:183:LEU:HD12	2.01	0.59
2:B:306:LEU:HB3	2:B:346:ILE:HG22	1.85	0.59
2:B:378:PHE:C	2:B:379:LEU:HD13	2.26	0.59
2:B:418:PHE:O	2:B:419:VAL:HG23	2.03	0.59
1:A:131:LYS:HE3	1:A:131:LYS:O	2.02	0.58
2:B:301:ARG:HD3	2:B:374:ASN:HA	1.85	0.58
1:A:148:LEU:C	1:A:149:ILE:HG13	2.27	0.58
1:A:221:LYS:HZ3	1:A:221:LYS:CA	2.17	0.58
1:A:192:LYS:HB2	1:A:203:TYR:CD2	2.38	0.58
1:A:109:LEU:N	1:A:162:PHE:O	2.37	0.58
1:A:94:LYS:HB3	1:A:95:PRO:HD2	1.85	0.58
1:A:117:ALA:HB2	1:A:157:LEU:HD13	1.85	0.58
1:A:221:LYS:HA	1:A:221:LYS:NZ	2.19	0.58
2:B:295:VAL:HG22	2:B:380:ALA:HB3	1.84	0.58
2:B:378:PHE:CE2	2:B:417:TYR:CD1	2.92	0.58
2:B:382:HIS:HD2	2:B:414:LYS:HA	1.68	0.58
1:A:192:LYS:HB2	1:A:203:TYR:CG	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:TYR:O	2:B:264:LYS:HA	2.04	0.57
1:A:114:GLU:O	1:A:114:GLU:HG3	2.03	0.57
1:A:151:PRO:O	1:A:153:ASN:N	2.38	0.57
2:B:290:GLU:N	2:B:361:ASP:OD1	2.33	0.57
2:B:378:PHE:CZ	2:B:417:TYR:HD1	2.23	0.57
1:A:58:THR:HG21	1:A:61:LYS:HB2	1.86	0.57
1:A:79:LYS:HE3	2:B:321:GLU:HB2	1.87	0.57
2:B:262:TYR:C	2:B:289:ASN:ND2	2.63	0.57
1:A:165:THR:OG1	1:A:170:GLY:N	2.26	0.57
1:A:69:LEU:HA	1:A:89:LEU:CD1	2.34	0.57
1:A:97:THR:CG2	1:A:221:LYS:NZ	2.68	0.57
1:A:131:LYS:HB3	2:B:241:THR:HG23	1.86	0.57
1:A:144:THR:HG22	1:A:145:PRO:N	2.18	0.57
1:A:56:PHE:CE2	1:A:90:GLU:HG3	2.40	0.57
1:A:207:GLU:CG	1:A:211:LEU:HD23	2.35	0.57
2:B:313:ALA:HB2	2:B:362:LEU:HD13	1.85	0.57
2:B:396:ASP:HB3	2:B:402:SER:OG	2.05	0.57
1:A:97:THR:HG22	1:A:221:LYS:HZ1	1.70	0.57
1:A:223:PRO:HD2	1:A:224:LYS:H	1.70	0.57
1:A:213:GLU:O	1:A:215:GLN:N	2.37	0.56
2:B:262:TYR:HB3	2:B:292:ALA:HB2	1.87	0.56
2:B:314:GLU:HA	2:B:339:THR:HA	1.87	0.56
1:A:51:PHE:O	2:B:347:VAL:HG23	2.05	0.56
2:B:269:THR:HA	2:B:282:LEU:CD1	2.35	0.56
2:B:270:PRO:O	2:B:277:ARG:HG2	2.06	0.56
2:B:396:ASP:HA	2:B:402:SER:HA	1.86	0.56
2:B:288:MET:HG2	2:B:292:ALA:HB3	1.87	0.56
2:B:413:GLN:OE1	2:B:415:GLU:HB2	2.06	0.56
1:A:110:VAL:CG1	1:A:159:ILE:HG23	2.35	0.56
2:B:249:PHE:N	2:B:249:PHE:CD1	2.74	0.56
1:A:97:THR:HG23	1:A:221:LYS:NZ	2.20	0.56
1:A:149:ILE:HG22	1:A:150:ASN:N	2.20	0.56
2:B:378:PHE:CE2	2:B:417:TYR:HD1	2.24	0.56
1:A:69:LEU:HD21	1:A:87:ARG:CZ	2.36	0.56
2:B:243:SER:O	2:B:245:GLN:N	2.38	0.56
1:A:60:PHE:CE2	1:A:218:VAL:CB	2.89	0.55
1:A:83:LEU:CA	1:A:86:TYR:HD2	2.20	0.55
1:A:85:ASP:OD1	1:A:85:ASP:N	2.38	0.55
1:A:108:LEU:CB	1:A:140:ILE:CG2	2.79	0.55
2:B:332:GLN:OE1	2:B:332:GLN:CA	2.54	0.55
1:A:213:GLU:O	1:A:215:GLN:OE1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:PHE:O	2:B:355:ALA:HB1	2.06	0.55
1:A:79:LYS:CE	2:B:321:GLU:HB2	2.38	0.54
1:A:104:SER:O	1:A:143:GLY:N	2.34	0.54
1:A:133:ASP:O	1:A:136:ASP:N	2.40	0.54
2:B:276:LEU:O	2:B:279:LEU:N	2.30	0.54
2:B:295:VAL:HB	2:B:417:TYR:O	2.08	0.54
1:A:70:LEU:CD2	2:B:345:ILE:HD13	2.35	0.54
1:A:110:VAL:C	1:A:111:LEU:HD13	2.32	0.54
1:A:98:LEU:HD13	1:A:149:ILE:CG1	2.38	0.54
1:A:110:VAL:HG12	1:A:159:ILE:HD12	1.88	0.54
1:A:179:SER:OG	1:A:185:SER:N	2.41	0.53
2:B:257:ILE:HG12	2:B:265:LEU:O	2.07	0.53
2:B:262:TYR:O	2:B:289:ASN:HB2	2.08	0.53
1:A:222:MET:HE2	1:A:224:LYS:CD	2.38	0.53
2:B:410:LEU:HD22	2:B:410:LEU:N	2.23	0.53
2:B:276:LEU:O	2:B:277:ARG:C	2.50	0.53
1:A:94:LYS:HG2	1:A:156:ASN:OD1	2.08	0.53
1:A:72:ARG:HB2	1:A:87:ARG:CZ	2.39	0.53
1:A:202:PRO:C	1:A:204:ASP:H	2.16	0.53
1:A:70:LEU:CD2	1:A:88:VAL:HG11	2.38	0.53
1:A:98:LEU:HD13	1:A:149:ILE:HG12	1.91	0.53
1:A:179:SER:HB3	1:A:184:PRO:CA	2.33	0.53
2:B:387:ILE:O	2:B:390:ILE:HG13	2.09	0.53
1:A:110:VAL:HG11	1:A:159:ILE:HD12	1.91	0.52
2:B:303:THR:HA	2:B:348:ILE:O	2.08	0.52
2:B:396:ASP:OD1	2:B:396:ASP:N	2.28	0.52
2:B:328:LEU:HD12	2:B:328:LEU:H	1.74	0.52
2:B:422:GLN:N	2:B:423:PRO:HD3	2.22	0.52
1:A:83:LEU:HB3	1:A:86:TYR:HD2	1.74	0.52
1:A:121:LEU:HD12	1:A:128:ASP:HB2	1.91	0.52
2:B:286:LEU:C	2:B:287:GLN:CG	2.81	0.52
2:B:298:TYR:CE2	2:B:379:LEU:HD11	2.45	0.52
1:A:69:LEU:CB	1:A:89:LEU:HD11	2.40	0.52
2:B:315:VAL:HB	2:B:338:ALA:O	2.10	0.52
2:B:333:LEU:HG	2:B:333:LEU:O	2.10	0.52
2:B:416:SER:HG	2:B:417:TYR:H	1.58	0.52
2:B:332:GLN:OE1	2:B:333:LEU:N	2.38	0.52
2:B:295:VAL:O	2:B:297:HIS:HB3	2.10	0.52
1:A:117:ALA:N	1:A:132:LEU:O	2.43	0.51
1:A:210:LEU:HD23	1:A:210:LEU:O	2.10	0.51
1:A:109:LEU:O	1:A:161:LYS:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TYR:CE1	2:B:287:GLN:NE2	2.79	0.51
2:B:288:MET:HE1	2:B:293:LEU:C	2.35	0.51
2:B:367:ILE:HD12	2:B:367:ILE:N	2.26	0.51
1:A:82:ASN:C	1:A:84:ARG:H	2.18	0.51
1:A:111:LEU:HD12	1:A:137:ALA:HB2	1.91	0.51
2:B:335:ARG:NH1	2:B:337:ALA:CB	2.72	0.51
1:A:222:MET:HB3	1:A:223:PRO:HD2	1.92	0.51
2:B:378:PHE:HD2	2:B:384:GLU:HB3	1.76	0.51
1:A:220:VAL:HG13	1:A:221:LYS:N	2.26	0.51
1:A:72:ARG:HB2	1:A:87:ARG:NE	2.26	0.51
2:B:251:LEU:CD1	2:B:268:ILE:HD13	2.29	0.51
2:B:262:TYR:N	2:B:262:TYR:CD1	2.78	0.51
1:A:117:ALA:C	1:A:132:LEU:H	2.17	0.50
2:B:318:VAL:HG12	2:B:319:GLY:N	2.27	0.50
2:B:320:LEU:O	2:B:320:LEU:HD12	2.12	0.50
2:B:378:PHE:CZ	2:B:417:TYR:CD1	2.99	0.50
2:B:245:GLN:O	2:B:246:ASP:HB3	2.11	0.50
2:B:260:ASN:HD21	2:B:416:SER:CB	2.24	0.50
1:A:168:ARG:HB3	1:A:171:THR:HB	1.94	0.50
2:B:394:VAL:HG12	2:B:398:THR:OG1	2.12	0.50
2:B:324:GLN:NE2	2:B:324:GLN:HA	2.26	0.49
1:A:113:LEU:O	1:A:114:GLU:CB	2.61	0.49
2:B:294:PHE:O	2:B:355:ALA:CB	2.61	0.49
1:A:112:VAL:HG13	1:A:159:ILE:HD13	1.95	0.49
1:A:72:ARG:HH12	1:A:171:THR:H	1.56	0.49
1:A:122:VAL:HG23	1:A:127:ARG:CA	2.40	0.49
2:B:297:HIS:O	2:B:353:PRO:HA	2.12	0.49
2:B:357:LYS:CG	2:B:358:ALA:N	2.76	0.49
1:A:148:LEU:O	1:A:149:ILE:HG13	2.12	0.49
2:B:357:LYS:HG2	2:B:358:ALA:N	2.27	0.48
1:A:221:LYS:CA	1:A:221:LYS:NZ	2.74	0.48
1:A:60:PHE:CE1	1:A:219:ILE:HD12	2.48	0.48
1:A:69:LEU:HA	1:A:89:LEU:HD12	1.95	0.48
1:A:222:MET:HE1	1:A:224:LYS:NZ	2.28	0.48
2:B:322:GLN:NE2	2:B:324:GLN:CB	2.72	0.48
2:B:420:ASP:CG	2:B:422:GLN:HB2	2.39	0.48
1:A:148:LEU:HD12	1:A:149:ILE:N	2.29	0.48
1:A:176:PHE:N	1:A:176:PHE:CD1	2.82	0.48
1:A:196:GLU:HG2	1:A:202:PRO:HA	1.96	0.48
2:B:265:LEU:HG	2:B:285:CYS:O	2.13	0.48
2:B:288:MET:HE1	2:B:294:PHE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:LEU:HD23	2:B:357:LYS:O	2.14	0.48
1:A:85:ASP:HA	1:A:170:GLY:HA2	1.95	0.48
1:A:103:HIS:HB2	1:A:144:THR:O	2.14	0.48
2:B:313:ALA:C	2:B:339:THR:HG23	2.39	0.48
2:B:324:GLN:NE2	2:B:324:GLN:CA	2.77	0.48
2:B:387:ILE:C	2:B:389:GLN:N	2.71	0.48
1:A:114:GLU:CG	1:A:158:ARG:HB2	2.44	0.48
1:A:108:LEU:CD1	1:A:146:PHE:CE2	2.97	0.48
2:B:257:ILE:HG13	2:B:258:TYR:CD2	2.49	0.47
2:B:317:LEU:HB3	2:B:336:TYR:HB2	1.97	0.47
1:A:83:LEU:HD21	2:B:369:VAL:HG21	1.96	0.47
2:B:264:LYS:O	2:B:286:LEU:HD22	2.14	0.47
2:B:415:GLU:CB	2:B:419:VAL:HG22	2.44	0.47
2:B:256:PRO:HD3	2:B:266:TYR:CE1	2.49	0.47
1:A:71:GLN:HA	1:A:87:ARG:HH12	1.79	0.47
1:A:118:ILE:HA	1:A:131:LYS:HA	1.95	0.47
2:B:328:LEU:CD1	2:B:329:GLU:N	2.78	0.47
1:A:76:ASP:OD1	1:A:76:ASP:N	2.48	0.47
1:A:222:MET:HB3	1:A:223:PRO:CD	2.45	0.47
2:B:306:LEU:HB3	2:B:346:ILE:CG2	2.44	0.47
1:A:54:ASN:OD1	1:A:54:ASN:N	2.48	0.47
1:A:120:VAL:HG12	1:A:127:ARG:HG2	1.97	0.47
2:B:352:PHE:CD1	2:B:352:PHE:N	2.83	0.47
2:B:257:ILE:CD1	2:B:258:TYR:CD2	2.99	0.46
2:B:354:VAL:CG2	2:B:355:ALA:N	2.78	0.46
2:B:270:PRO:O	2:B:277:ARG:NH1	2.43	0.46
2:B:268:ILE:HG21	2:B:273:ASN:HB2	1.96	0.46
1:A:44:ALA:HB3	1:A:71:GLN:NE2	2.30	0.46
2:B:257:ILE:CG1	2:B:258:TYR:CD2	2.98	0.46
2:B:305:ILE:O	2:B:366:GLY:HA2	2.15	0.46
1:A:79:LYS:NZ	2:B:321:GLU:HB2	2.30	0.46
2:B:403:GLY:O	2:B:407:GLU:CB	2.63	0.46
2:B:294:PHE:HE1	2:B:417:TYR:HB3	1.80	0.46
2:B:396:ASP:CB	2:B:402:SER:OG	2.64	0.46
2:B:243:SER:O	2:B:245:GLN:NE2	2.35	0.46
1:A:111:LEU:HD12	1:A:137:ALA:CB	2.46	0.46
1:A:60:PHE:CE2	1:A:218:VAL:CG2	2.99	0.46
2:B:324:GLN:C	2:B:325:GLN:OE1	2.59	0.46
2:B:422:GLN:HA	2:B:423:PRO:HD2	1.51	0.46
1:A:119:LEU:HB2	1:A:132:LEU:HD12	1.98	0.45
1:A:136:ASP:OD1	2:B:252:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LYS:HA	1:A:221:LYS:HZ2	1.81	0.45
2:B:259:SER:HB3	2:B:264:LYS:HG2	1.97	0.45
2:B:390:ILE:HG22	2:B:391:PRO:HD2	1.98	0.45
2:B:396:ASP:CG	2:B:402:SER:OG	2.59	0.45
1:A:108:LEU:CD1	1:A:146:PHE:HE2	2.29	0.45
1:A:180:THR:HB	1:A:217:GLY:O	2.16	0.45
2:B:260:ASN:C	2:B:262:TYR:N	2.74	0.45
2:B:398:THR:HG22	2:B:399:PHE:CE1	2.51	0.45
1:A:72:ARG:NH1	1:A:170:GLY:CA	2.78	0.45
1:A:169:PRO:C	1:A:171:THR:H	2.25	0.45
1:A:206:ILE:O	1:A:210:LEU:HB2	2.16	0.45
1:A:196:GLU:OE2	1:A:202:PRO:HA	2.17	0.45
2:B:306:LEU:HD22	2:B:348:ILE:HD12	1.98	0.45
2:B:304:VAL:HG13	2:B:305:ILE:O	2.17	0.45
1:A:140:ILE:HD13	1:A:140:ILE:HG21	1.72	0.45
1:A:223:PRO:CD	1:A:224:LYS:N	2.79	0.45
2:B:260:ASN:OD1	2:B:262:TYR:CD1	2.70	0.45
1:A:224:LYS:HG3	1:A:224:LYS:O	2.17	0.45
1:A:49:TYR:CZ	1:A:79:LYS:CD	3.00	0.45
2:B:405:GLU:O	2:B:409:LEU:HD12	2.16	0.45
1:A:60:PHE:CD1	1:A:60:PHE:C	2.95	0.44
2:B:256:PRO:HG2	2:B:259:SER:OG	2.18	0.44
2:B:340:LEU:O	2:B:341:SER:OG	2.35	0.44
1:A:62:ASN:ND2	1:A:216:GLU:HB2	2.28	0.44
1:A:103:HIS:CB	1:A:144:THR:O	2.65	0.44
1:A:150:ASN:OD1	1:A:157:LEU:CB	2.64	0.44
2:B:260:ASN:C	2:B:262:TYR:H	2.25	0.44
2:B:356:LEU:HD23	2:B:357:LYS:C	2.41	0.44
1:A:58:THR:O	1:A:58:THR:HG22	2.17	0.44
1:A:221:LYS:CB	1:A:221:LYS:NZ	2.76	0.44
2:B:369:VAL:O	2:B:370:ASN:C	2.60	0.44
1:A:69:LEU:HA	1:A:89:LEU:HD11	2.00	0.44
1:A:123:ASN:CB	1:A:124:PRO:CD	2.85	0.44
2:B:378:PHE:O	2:B:385:ASN:OD1	2.35	0.44
1:A:128:ASP:OD2	1:A:130:TYR:OH	2.24	0.44
1:A:129:THR:HB	2:B:242:LEU:HD13	1.99	0.44
2:B:386:VAL:O	2:B:389:GLN:N	2.49	0.44
1:A:52:ARG:HH21	1:A:54:ASN:ND2	2.16	0.44
1:A:71:GLN:C	1:A:87:ARG:NH1	2.76	0.44
1:A:110:VAL:HG12	1:A:159:ILE:CD1	2.47	0.44
2:B:328:LEU:C	2:B:330:SER:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:THR:HG23	2:B:349:PRO:HA	2.00	0.43
1:A:97:THR:HG22	1:A:221:LYS:NZ	2.32	0.43
1:A:100:LEU:HG	1:A:218:VAL:O	2.18	0.43
1:A:111:LEU:HD13	1:A:111:LEU:N	2.33	0.43
1:A:202:PRO:C	1:A:204:ASP:N	2.76	0.43
2:B:253:SER:CB	2:B:266:TYR:CD2	2.98	0.43
2:B:392:ARG:O	2:B:395:SER:OG	2.29	0.43
1:A:83:LEU:HD22	2:B:369:VAL:HG21	1.99	0.43
1:A:97:THR:HA	1:A:220:VAL:O	2.18	0.43
1:A:118:ILE:HD13	1:A:131:LYS:HA	2.01	0.43
1:A:183:LEU:HA	1:A:184:PRO:HD3	1.54	0.43
1:A:199:TYR:CD2	1:A:206:ILE:HG12	2.53	0.43
2:B:281:ILE:HA	2:B:368:GLY:O	2.18	0.43
2:B:251:LEU:C	2:B:251:LEU:HD12	2.43	0.43
2:B:340:LEU:HD22	2:B:344:ASP:HB3	2.00	0.43
1:A:69:LEU:CD2	1:A:87:ARG:NH1	2.75	0.43
2:B:268:ILE:CG2	2:B:273:ASN:HB2	2.48	0.43
2:B:276:LEU:C	2:B:278:ASP:N	2.77	0.43
1:A:49:TYR:CZ	1:A:79:LYS:HD2	2.51	0.43
1:A:183:LEU:O	1:A:184:PRO:O	2.37	0.43
1:A:202:PRO:HB2	1:A:204:ASP:OD2	2.18	0.43
1:A:207:GLU:O	1:A:209:THR:N	2.51	0.43
2:B:354:VAL:HG22	2:B:355:ALA:N	2.32	0.43
1:A:52:ARG:NH2	1:A:54:ASN:ND2	2.66	0.43
1:A:102:HIS:HB3	1:A:176:PHE:HA	2.00	0.43
2:B:286:LEU:O	2:B:287:GLN:HG2	2.19	0.43
2:B:270:PRO:CB	2:B:277:ARG:CA	2.89	0.43
2:B:288:MET:CE	2:B:293:LEU:N	2.81	0.43
2:B:349:PRO:HB2	2:B:352:PHE:CD1	2.54	0.43
1:A:83:LEU:CB	1:A:86:TYR:HD2	2.31	0.43
2:B:386:VAL:CG1	2:B:387:ILE:N	2.82	0.43
2:B:247:LYS:H	2:B:247:LYS:HG3	1.00	0.42
2:B:315:VAL:HG21	2:B:346:ILE:HD13	2.00	0.42
2:B:253:SER:HB3	2:B:266:TYR:HD2	1.80	0.42
1:A:70:LEU:CD2	1:A:88:VAL:CG1	2.97	0.42
1:A:207:GLU:OE2	1:A:211:LEU:CD2	2.67	0.42
2:B:295:VAL:O	2:B:296:PRO:C	2.62	0.42
2:B:322:GLN:HE21	2:B:324:GLN:HB3	1.80	0.42
2:B:324:GLN:CA	2:B:324:GLN:HE21	2.32	0.42
2:B:420:ASP:OD2	2:B:422:GLN:HB2	2.19	0.42
1:A:47:ASN:CB	1:A:48:PRO:CD	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLU:C	1:A:215:GLN:O	2.63	0.42
1:A:224:LYS:CD	1:A:224:LYS:C	2.93	0.42
1:A:56:PHE:N	1:A:56:PHE:CD1	2.88	0.42
2:B:273:ASN:OD1	2:B:274:SER:N	2.53	0.42
2:B:421:GLY:O	2:B:423:PRO:N	2.52	0.42
1:A:111:LEU:CD1	1:A:137:ALA:CB	2.97	0.42
1:A:117:ALA:HB2	1:A:157:LEU:CD1	2.49	0.42
1:A:155:GLN:HG2	1:A:156:ASN:ND2	2.35	0.42
2:B:251:LEU:CD1	2:B:268:ILE:CD1	2.94	0.42
2:B:387:ILE:C	2:B:389:GLN:H	2.28	0.42
2:B:415:GLU:CB	2:B:419:VAL:CG2	2.97	0.42
1:A:60:PHE:CE2	1:A:218:VAL:HG23	2.54	0.42
1:A:109:LEU:HB3	1:A:162:PHE:HB3	1.99	0.42
2:B:308:ALA:HB3	2:B:341:SER:O	2.20	0.42
1:A:60:PHE:CD2	1:A:218:VAL:HB	2.55	0.42
1:A:85:ASP:HA	1:A:170:GLY:N	2.35	0.42
1:A:110:VAL:HG13	1:A:159:ILE:CG2	2.41	0.42
1:A:215:GLN:C	1:A:217:GLY:N	2.76	0.42
2:B:298:TYR:CD1	2:B:298:TYR:C	2.97	0.42
2:B:403:GLY:O	2:B:407:GLU:HB2	2.19	0.42
1:A:108:LEU:HB2	1:A:140:ILE:O	2.20	0.42
2:B:257:ILE:HD12	2:B:258:TYR:HE2	1.76	0.42
2:B:293:LEU:O	2:B:418:PHE:HA	2.20	0.42
2:B:342:GLU:O	2:B:342:GLU:HG2	2.20	0.42
1:A:79:LYS:C	1:A:80:LEU:HD23	2.45	0.41
2:B:317:LEU:HD23	2:B:336:TYR:HB2	2.02	0.41
1:A:108:LEU:HA	1:A:162:PHE:O	2.19	0.41
2:B:337:ALA:O	2:B:338:ALA:HB2	2.21	0.41
1:A:131:LYS:HB3	2:B:241:THR:CG2	2.50	0.41
1:A:137:ALA:O	2:B:250:ASN:ND2	2.53	0.41
1:A:141:GLN:O	1:A:142:ALA:O	2.37	0.41
1:A:144:THR:CG2	1:A:145:PRO:N	2.82	0.41
1:A:212:GLN:HB2	1:A:213:GLU:H	1.71	0.41
1:A:97:THR:HG23	1:A:221:LYS:HZ1	1.78	0.41
1:A:176:PHE:CE2	1:A:218:VAL:CG1	3.03	0.41
1:A:207:GLU:CD	1:A:211:LEU:HD23	2.45	0.41
2:B:253:SER:CB	2:B:266:TYR:HD2	2.34	0.41
2:B:260:ASN:ND2	2:B:416:SER:HG	2.11	0.41
2:B:360:SER:C	2:B:362:LEU:N	2.78	0.41
1:A:83:LEU:HB3	1:A:86:TYR:CD2	2.55	0.41
2:B:261:ASN:C	2:B:261:ASN:ND2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:ILE:O	2:B:283:LEU:N	2.47	0.41
1:A:63:GLN:O	1:A:64:HIS:CG	2.73	0.41
1:A:215:GLN:H	1:A:215:GLN:CD	2.27	0.41
1:A:49:TYR:CE1	1:A:79:LYS:CD	2.95	0.41
1:A:49:TYR:CZ	1:A:79:LYS:CG	3.04	0.41
1:A:99:LEU:C	1:A:99:LEU:HD12	2.46	0.41
1:A:192:LYS:HA	1:A:203:TYR:CE1	2.56	0.41
2:B:372:GLU:O	2:B:372:GLU:HG2	2.19	0.41
2:B:378:PHE:CD2	2:B:384:GLU:CB	2.98	0.41
2:B:245:GLN:H	2:B:245:GLN:HG2	1.71	0.41
1:A:149:ILE:HG22	1:A:150:ASN:H	1.82	0.40
1:A:149:ILE:CG2	1:A:150:ASN:N	2.83	0.40
1:A:152:ASP:OD1	1:A:152:ASP:N	2.30	0.40
2:B:415:GLU:HB2	2:B:419:VAL:HG22	2.03	0.40
2:B:352:PHE:HA	2:B:353:PRO:HD3	1.77	0.40
2:B:263:GLY:HA2	2:B:287:GLN:O	2.21	0.40
1:A:70:LEU:HD12	1:A:70:LEU:HA	1.90	0.40
1:A:112:VAL:C	1:A:114:GLU:H	2.30	0.40
1:A:118:ILE:O	1:A:118:ILE:HG22	2.21	0.40
1:A:165:THR:H	1:A:165:THR:HG23	1.68	0.40
1:A:193:ASN:CB	1:A:194:PHE:CD1	3.00	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%)	126 (70%)	30 (17%)	23 (13%)	0	0
2	B	182/184 (99%)	130 (71%)	35 (19%)	17 (9%)	0	0
All	All	361/365 (99%)	256 (71%)	65 (18%)	40 (11%)	0	0

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	64	HIS
1	A	83	LEU
1	A	96	ASN
1	A	114	GLU
1	A	123	ASN
1	A	142	ALA
1	A	152	ASP
1	A	154	ASN
1	A	184	PRO
1	A	207	GLU
1	A	215	GLN
1	A	216	GLU
2	B	244	SER
2	B	246	ASP
2	B	248	PRO
2	B	249	PHE
2	B	277	ARG
2	B	290	GLU
2	B	350	SER
2	B	360	SER
2	B	404	GLU
1	A	45	GLN
1	A	153	ASN
1	A	208	GLN
1	A	209	THR
2	B	296	PRO
1	A	193	ASN
1	A	223	PRO
2	B	289	ASN
1	A	202	PRO
2	B	291	GLY
2	B	422	GLN
1	A	124	PRO
1	A	136	ASP
2	B	330	SER
2	B	343	GLY
2	B	329	GLU
2	B	388	ARG
1	A	47	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/167 (100%)	97 (58%)	70 (42%)	0	0
2	B	161/161 (100%)	84 (52%)	77 (48%)	0	0
All	All	328/328 (100%)	181 (55%)	147 (45%)	0	0

All (147) 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	50	LEU
1	A	54	ASN
1	A	57	LEU
1	A	63	GLN
1	A	67	LEU
1	A	76	ASP
1	A	79	LYS
1	A	81	GLU
1	A	82	ASN
1	A	83	LEU
1	A	85	ASP
1	A	88	VAL
1	A	89	LEU
1	A	94	LYS
1	A	97	THR
1	A	98	LEU
1	A	99	LEU
1	A	102	HIS
1	A	104	SER
1	A	109	LEU
1	A	111	LEU
1	A	112	VAL
1	A	120	VAL

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Mol	Chain	Res	Type
1	A	121	LEU
1	A	122	VAL
1	A	129	THR
1	A	130	TYR
1	A	131	LYS
1	A	139	LYS
1	A	141	GLN
1	A	152	ASP
1	A	154	ASN
1	A	157	LEU
1	A	158	ARG
1	A	159	ILE
1	A	167	ARG
1	A	168	ARG
1	A	171	THR
1	A	173	GLU
1	A	175	PHE
1	A	176	PHE
1	A	177	LEU
1	A	179	SER
1	A	180	THR
1	A	181	LYS
1	A	182	ARG
1	A	183	LEU
1	A	190	PHE
1	A	192	LYS
1	A	194	PHE
1	A	198	SER
1	A	200	ASP
1	A	201	SER
1	A	206	ILE
1	A	208	GLN
1	A	209	THR
1	A	212	GLN
1	A	213	GLU
1	A	214	GLU
1	A	215	GLN
1	A	216	GLU
1	A	218	VAL
1	A	220	VAL
1	A	221	LYS
1	A	222	MET

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Mol	Chain	Res	Type
1	A	224	LYS
2	B	241	THR
2	B	242	LEU
2	B	243	SER
2	B	245	GLN
2	B	246	ASP
2	B	247	LYS
2	B	249	PHE
2	B	250	ASN
2	B	253	SER
2	B	254	ARG
2	B	257	ILE
2	B	259	SER
2	B	260	ASN
2	B	261	ASN
2	B	262	TYR
2	B	265	LEU
2	B	271	GLU
2	B	272	LYS
2	B	274	SER
2	B	277	ARG
2	B	278	ASP
2	B	279	LEU
2	B	281	ILE
2	B	282	LEU
2	B	284	ASN
2	B	286	LEU
2	B	288	MET
2	B	290	GLU
2	B	293	LEU
2	B	294	PHE
2	B	295	VAL
2	B	299	ASN
2	B	305	ILE
2	B	306	LEU
2	B	307	VAL
2	B	310	GLU
2	B	314	GLU
2	B	316	GLU
2	B	320	LEU
2	B	321	GLU
2	B	324	GLN

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Mol	Chain	Res	Type
2	B	325	GLN
2	B	328	LEU
2	B	330	SER
2	B	331	MET
2	B	333	LEU
2	B	341	SER
2	B	345	ILE
2	B	347	VAL
2	B	351	SER
2	B	354	VAL
2	B	361	ASP
2	B	362	LEU
2	B	364	MET
2	B	365	VAL
2	B	369	VAL
2	B	372	GLU
2	B	374	ASN
2	B	375	GLU
2	B	376	ARG
2	B	377	ASN
2	B	379	LEU
2	B	382	HIS
2	B	383	LYS
2	B	384	GLU
2	B	386	VAL
2	B	387	ILE
2	B	390	ILE
2	B	392	ARG
2	B	393	GLN
2	B	395	SER
2	B	396	ASP
2	B	397	LEU
2	B	402	SER
2	B	407	GLU
2	B	414	LYS
2	B	419	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	62	ASN

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Mol	Chain	Res	Type
1	A	63	GLN
1	A	71	GLN
1	A	96	ASN
1	A	103	HIS
1	A	155	GLN
1	A	208	GLN
2	B	250	ASN
2	B	260	ASN
2	B	261	ASN
2	B	289	ASN
2	B	322	GLN
2	B	324	GLN
2	B	382	HIS
2	B	422	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-1.44	0 100 100	11, 25, 33, 37	0
2	B	184/184 (100%)	-1.44	0 100 100	11, 25, 35, 45	0
All	All	365/365 (100%)	-1.44	0 100 100	11, 25, 34, 45	0

There are no RSRZ outliers to report.

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.