Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:44 PM GMT

PDB ID	:	1CAW
Title	:	DETERMINATION OF THREE CRYSTAL STRUCTURES OF CANAVALIN BY MOLECULAR REPLACEMENT
Authors	:	Ko, T-P.; Ng, J.D.; Day, J.; Greenwood, A.; McPherson, A.
Deposited on	:	1993-06-02
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

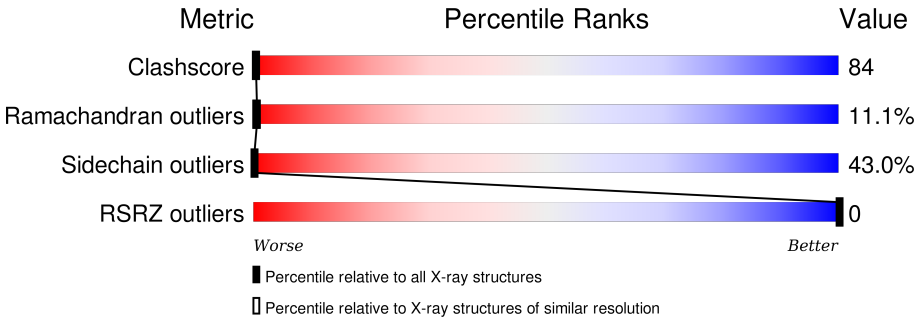
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	13% 41% 31% 14%
2	B	184	10% 46% 33% 11%

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.

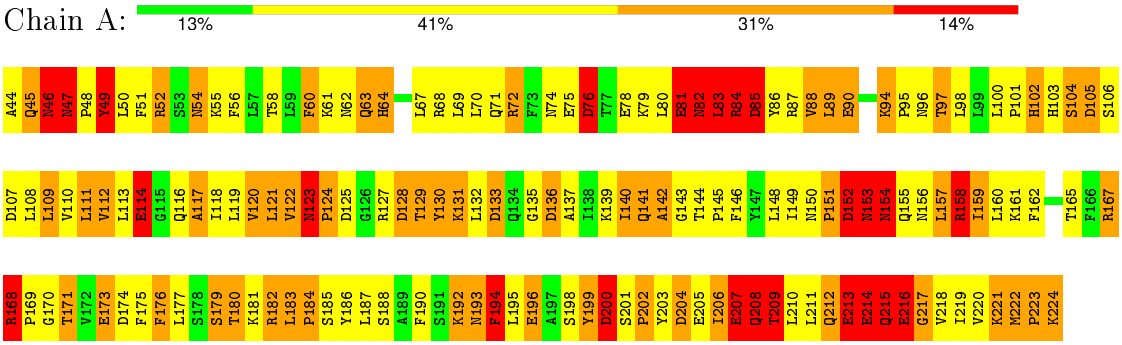
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	184	1450	902	255	289	4	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

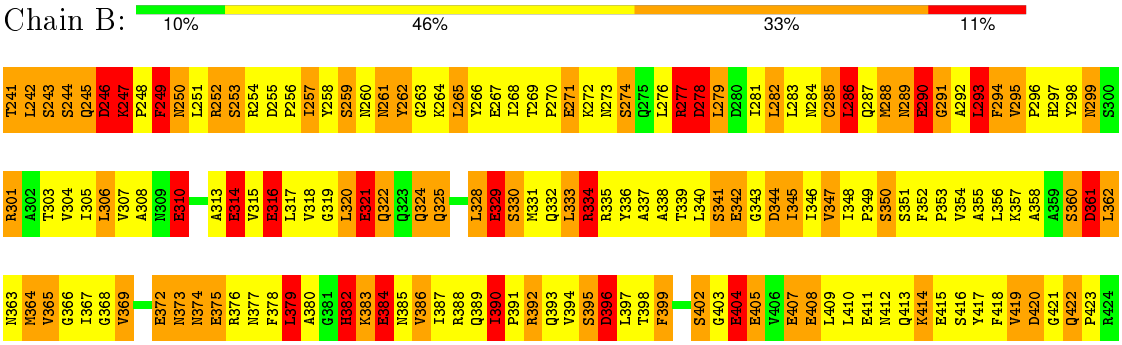
- Molecule 1: CANAVALIN

Chain A:



- Molecule 2: CANAVALIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	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 30.14 – 2.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 62.8 (30.14-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 2.57Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.194 , (Not available) 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 90.1	EDS
Estimated twinning fraction	0.436 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 10592 reflections	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.30	13/1511 (0.9%)	1.75	43/2046 (2.1%)
2	B	1.34	17/1472 (1.2%)	1.70	26/1992 (1.3%)
All	All	1.32	30/2983 (1.0%)	1.72	69/4038 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
2	B	1	1
All	All	2	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CD-OE2	10.77	1.37	1.25
2	B	411	GLU	CD-OE1	8.57	1.35	1.25
2	B	329	GLU	CD-OE2	8.08	1.34	1.25
2	B	271	GLU	CD-OE1	8.07	1.34	1.25
2	B	290	GLU	CD-OE1	7.75	1.34	1.25
1	A	205	GLU	CD-OE2	7.51	1.33	1.25
2	B	408	GLU	CD-OE2	7.41	1.33	1.25
1	A	114	GLU	CD-OE1	7.33	1.33	1.25
2	B	314	GLU	CD-OE2	7.23	1.33	1.25
1	A	207	GLU	CD-OE1	6.71	1.33	1.25
2	B	404	GLU	CD-OE1	6.63	1.32	1.25
2	B	267	GLU	CD-OE1	6.41	1.32	1.25
1	A	214	GLU	CD-OE1	6.34	1.32	1.25
2	B	321	GLU	CD-OE2	6.33	1.32	1.25
1	A	90	GLU	CD-OE1	6.21	1.32	1.25
1	A	213	GLU	CD-OE1	6.11	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	252	ARG	NE-CZ	6.00	1.40	1.33
1	A	196	GLU	CD-OE1	5.97	1.32	1.25
1	A	78	GLU	CD-OE2	5.96	1.32	1.25
1	A	81	GLU	CD-OE1	5.96	1.32	1.25
2	B	316	GLU	CD-OE2	5.86	1.32	1.25
2	B	375	GLU	CD-OE1	5.84	1.32	1.25
2	B	405	GLU	CD-OE1	5.72	1.31	1.25
2	B	310	GLU	CD-OE1	5.53	1.31	1.25
2	B	342	GLU	CD-OE1	5.46	1.31	1.25
2	B	384	GLU	CD-OE1	5.43	1.31	1.25
2	B	407	GLU	CD-OE2	5.43	1.31	1.25
1	A	75	GLU	CD-OE1	5.42	1.31	1.25
1	A	52	ARG	NE-CZ	5.39	1.40	1.33
1	A	173	GLU	CD-OE2	5.18	1.31	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	247	LYS	C-N-CD	-16.39	84.54	120.60
2	B	396	ASP	CB-CG-OD2	-10.06	109.24	118.30
2	B	334	ARG	NE-CZ-NH1	10.03	125.32	120.30
1	A	84	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	84	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	167	ARG	N-CA-CB	8.79	126.42	110.60
1	A	52	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	152	ASP	CB-CG-OD2	7.96	125.47	118.30
1	A	107	ASP	CB-CG-OD1	-7.91	111.19	118.30
1	A	153	ASN	N-CA-CB	7.63	124.34	110.60
1	A	85	ASP	CB-CG-OD1	-7.58	111.48	118.30
2	B	278	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	133	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	A	158	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	123	ASN	C-N-CD	-7.30	104.53	120.60
2	B	252	ARG	NE-CZ-NH1	7.29	123.94	120.30
2	B	334	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	105	ASP	CB-CG-OD2	7.13	124.71	118.30
2	B	379	LEU	N-CA-CB	6.92	124.24	110.40
1	A	200	ASP	CB-CG-OD2	6.91	124.52	118.30
2	B	384	GLU	CB-CA-C	6.91	124.22	110.40
1	A	76	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	204	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	204	ASP	CB-CG-OD1	-6.70	112.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	382	HIS	CA-CB-CG	-6.60	102.38	113.60
2	B	255	ASP	CB-CG-OD1	-6.55	112.40	118.30
2	B	344	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	174	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	85	ASP	CB-CG-OD2	6.40	124.06	118.30
2	B	246	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	49	TYR	CB-CG-CD2	-6.25	117.25	121.00
2	B	278	ASP	CB-CG-OD2	-6.19	112.73	118.30
2	B	246	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	154	ASN	N-CA-C	6.14	127.57	111.00
2	B	396	ASP	CB-CA-C	-6.11	98.18	110.40
1	A	105	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	49	TYR	CB-CA-C	5.99	122.38	110.40
1	A	125	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	A	128	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	128	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	101	PRO	N-CA-CB	5.90	110.38	103.30
2	B	344	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	A	72	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	49	TYR	CB-CG-CD1	5.82	124.49	121.00
1	A	200	ASP	N-CA-CB	5.72	120.91	110.60
1	A	200	ASP	CB-CG-OD1	-5.71	113.16	118.30
2	B	286	LEU	N-CA-CB	-5.69	99.02	110.40
2	B	322	GLN	N-CA-CB	5.67	120.80	110.60
1	A	168	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	B	293	LEU	CB-CA-C	5.63	120.91	110.20
2	B	246	ASP	N-CA-CB	5.61	120.70	110.60
1	A	82	ASN	N-CA-CB	5.50	120.50	110.60
1	A	217	GLY	N-CA-C	5.46	126.76	113.10
1	A	49	TYR	CA-CB-CG	5.45	123.76	113.40
2	B	390	ILE	N-CA-CB	5.41	123.24	110.80
1	A	194	PHE	CB-CA-C	5.40	121.20	110.40
2	B	399	PHE	CA-CB-CG	5.40	126.87	113.90
2	B	420	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	A	199	TYR	CB-CG-CD1	-5.33	117.80	121.00
2	B	383	LYS	O-C-N	5.32	131.21	122.70
2	B	244	SER	N-CA-CB	5.28	118.42	110.50
1	A	167	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	152	ASP	CB-CA-C	5.17	120.75	110.40
1	A	151	PRO	N-CA-CB	5.16	109.50	103.30
1	A	76	ASP	CB-CG-OD2	-5.13	113.69	118.30
2	B	361	ASP	CB-CG-OD1	-5.12	113.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	ILE	N-CA-CB	-5.11	99.04	110.80
1	A	117	ALA	N-CA-CB	5.10	117.24	110.10
1	A	125	ASP	CB-CG-OD2	5.02	122.82	118.30

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	264	0
2	B	1450	0	1425	247	0
All	All	2930	0	2898	490	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 84.

All (490) 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
2:B:286:LEU:C	2:B:286:LEU:HD13	1.69	1.12
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:286:LEU:C	2:B:286:LEU:CD1	2.37	0.93
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:72:ARG:NH1	1:A:171:THR:N	2.24	0.86
1:A:49:TYR:CE1	1:A:79:LYS:HD2	2.10	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:131:LYS:HE2	2:B:241:THR:CG2	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
1:A:108:LEU:CB	1:A:140:ILE:HG23	2.10	0.81
2:B:414:LYS:HD3	2:B:414:LYS:H	1.44	0.81
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
2:B:270:PRO:HB3	2:B:277:ARG:N	1.97	0.80
1:A:155:GLN:HG2	1:A:156:ASN:H	1.45	0.80
1:A:116:GLN:O	1:A:151:PRO:HD2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:THR:O	2:B:369:VAL:HG23	1.81	0.79
1:A:47:ASN:CG	1:A:48:PRO:HD2	2.02	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: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:261:ASN:C	2:B:261:ASN:HD22	1.88	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:110:VAL:CG1	1:A:159:ILE:HD12	2.16	0.75
1:A:74:ASN:HB2	1:A:81:GLU:OE2	1.86	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:N	2:B:379:LEU:HD13	2.02	0.75
2:B:262:TYR:C	2:B:289:ASN:HD22	1.89	0.75
1:A:87:ARG:HG2	1:A:170:GLY:O	1.86	0.75
2:B:315:VAL:HG11	2:B:346:ILE:HD13	1.66	0.74
1:A:79:LYS:O	1:A:80:LEU:HD23	1.87	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
2:B:322:GLN:O	2:B:331:MET:HG3	1.87	0.72
1:A:144:THR:HG22	1:A:145:PRO:O	1.88	0.72
2:B:279:LEU:HD23	2:B:279:LEU:N	2.03	0.72
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	2:B:249:PHE:HD1	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:CD	2:B:414:LYS:H	2.01	0.68
2:B:261:ASN:O	2:B:289:ASN:ND2	2.27	0.68
1:A:79:LYS:HE3	2:B:321:GLU:CD	2.13	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:278:ASP:C	2:B:279:LEU:HD23	2.15	0.67
1:A:221:LYS:HZ3	1:A:221:LYS:CA	2.07	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: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
1:A:83:LEU:CD2	2:B:369:VAL:HG21	2.26	0.66
1:A:81:GLU:O	1:A:84:ARG:HG2	1.95	0.66
1:A:221:LYS:HZ3	1:A:221:LYS:CB	2.08	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
2:B:257:ILE:CD1	2:B:265:LEU:HD23	2.23	0.65
1:A:49:TYR:OH	1:A:79:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:221:LYS:HZ3	1:A:221:LYS:HB2	1.63	0.64
2:B:360:SER:O	2:B:362:LEU:N	2.31	0.64
2:B:378:PHE:HD2	2:B:384:GLU:CB	2.10	0.64
1:A:47:ASN:ND2	1:A:48:PRO:HD2	2.12	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:185:SER:OG	1:A:186:TYR:N	2.28	0.63
1:A:70:LEU:O	1:A:87:ARG:NH1	2.30	0.63
2:B:251:LEU:HD13	2:B:268:ILE:CD1	2.25	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: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:133:ASP:O	1:A:136:ASP:HB2	1.99	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:223:PRO:CD	1:A:224:LYS:H	2.13	0.62
1:A:213:GLU:OE1	1:A:213:GLU:O	2.18	0.61
2:B:410:LEU:H	2:B:410:LEU:HD22	1.64	0.61
2:B:262:TYR:CA	2:B:289:ASN:HD22	2.13	0.61
2:B:313:ALA:O	2:B:339:THR:HA	2.00	0.61
1:A:196:GLU:O	1:A:200:ASP:HA	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:ALA:HB2	2:B:362:LEU:HD11	1.82	0.60
1:A:221:LYS:C	1:A:222:MET:HG3	2.22	0.60
1:A:110:VAL:O	1:A:137:ALA:HA	2.02	0.60
1:A:194:PHE:N	1:A:194:PHE:CD1	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:112:VAL:HG13	1:A:159:ILE:HD11	1.82	0.59
1:A:47:ASN:CB	1:A:48:PRO:HD2	2.32	0.59
1:A:150:ASN:OD1	1:A:157:LEU:HB2	2.02	0.59
2:B:288:MET:HE2	2:B:292:ALA:C	2.23	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: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: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:144:THR:HG22	1:A:145:PRO:N	2.18	0.58
1:A:117:ALA:HB2	1:A:157:LEU:HD13	1.85	0.58
2:B:295:VAL:HG22	2:B:380:ALA:HB3	1.84	0.58
1:A:221:LYS:NZ	1:A:221:LYS:HA	2.19	0.58
2:B:382:HIS:HD2	2:B:414:LYS:HA	1.68	0.58
2:B:378:PHE:CE2	2:B:417:TYR:CD1	2.92	0.58
2:B:258:TYR:O	2:B:264:LYS:HA	2.04	0.57
1:A:192:LYS:HB2	1:A:203:TYR:CG	2.39	0.57
1:A:114:GLU:O	1:A:114:GLU:HG3	2.03	0.57
1:A:72:ARG:NH1	1:A:170:GLY:C	2.57	0.57
2:B:378:PHE:CZ	2:B:417:TYR:HD1	2.23	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
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
1:A:165:THR:OG1	1:A:170:GLY:N	2.26	0.57
1:A:131:LYS:HB3	2:B:241:THR:HG23	1.86	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:208:GLN:O	1:A:209:THR:OG1	2.17	0.57
1:A:56:PHE:CE2	1:A:90:GLU:HG3	2.40	0.57
1:A:213:GLU:O	1:A:214:GLU:C	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:ASP:HB3	2:B:402:SER:OG	2.05	0.57
2:B:313:ALA:HB2	2:B:362:LEU:HD13	1.85	0.57
1:A:207:GLU:CG	1:A:211:LEU:HD23	2.35	0.57
1:A:223:PRO:HD2	1:A:224:LYS:H	1.70	0.57
2:B:262:TYR:HB3	2:B:292:ALA:HB2	1.87	0.56
1:A:213:GLU:O	1:A:215:GLN:N	2.37	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
1:A:97:THR:CG2	1:A:221:LYS:HZ1	2.18	0.56
2:B:286:LEU:C	2:B:287:GLN:HG2	2.24	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:CD1	2:B:249:PHE:N	2.74	0.56
2:B:378:PHE:CE2	2:B:417:TYR:HD1	2.24	0.56
1:A:149:ILE:HG22	1:A:150:ASN:N	2.20	0.56
1:A:97:THR:HG23	1:A:221:LYS:NZ	2.20	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:45:GLN:CD	1:A:46:ASN:H	2.10	0.55
1:A:108:LEU:CB	1:A:140:ILE:CG2	2.79	0.55
1:A:85:ASP:N	1:A:85:ASP:OD1	2.38	0.55
2:B:332:GLN:CA	2:B:332:GLN:OE1	2.54	0.55
1:A:213:GLU:O	1:A:215:GLN:OE1	2.25	0.55
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:135:GLY:O	1:A:136:ASP:C	2.46	0.54
2:B:276:LEU:O	2:B:279:LEU:N	2.30	0.54
1:A:133:ASP:O	1:A:136:ASP:N	2.40	0.54
2:B:378:PHE:C	2:B:379:LEU:HD13	2.26	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:HG12	1:A:159:ILE:HD12	1.88	0.54
1:A:148:LEU:C	1:A:149:ILE:HG13	2.27	0.54
1:A:98:LEU:HD13	1:A:149:ILE:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:HG12	2:B:265:LEU:O	2.07	0.53
1:A:179:SER:OG	1:A:185:SER:N	2.41	0.53
2:B:262:TYR:O	2:B:289:ASN:HB2	2.08	0.53
2:B:410:LEU:N	2:B:410:LEU:HD22	2.23	0.53
1:A:94:LYS:HG2	1:A:156:ASN:OD1	2.08	0.53
1:A:222:MET:HE1	1:A:224:LYS:CD	2.38	0.53
1:A:72:ARG:HB2	1:A:87:ARG:CZ	2.39	0.53
1:A:179:SER:HB3	1:A:184:PRO:CA	2.33	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
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:N	2:B:396:ASP:OD1	2.28	0.52
2:B:328:LEU:H	2:B:328:LEU:HD12	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: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:416:SER:HG	2:B:417:TYR:H	1.58	0.52
2:B:333:LEU:O	2:B:333:LEU:HG	2.10	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:O	1:A:210:LEU:HD23	2.10	0.51
1:A:109:LEU:O	1:A:161:LYS:HA	2.10	0.51
2:B:266:TYR:CE1	2:B:287:GLN:NE2	2.79	0.51
2:B:392:ARG:O	2:B:395:SER:OG	2.29	0.51
2:B:367:ILE:N	2:B:367:ILE:HD12	2.26	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
2:B:378:PHE:HD2	2:B:384:GLU:HB3	1.76	0.51
1:A:222:MET:HB3	1:A:223:PRO:HD2	1.92	0.51
1:A:220:VAL:HG13	1:A:221:LYS:N	2.26	0.51
2:B:251:LEU:CD1	2:B:268:ILE:HD13	2.29	0.51
1:A:72:ARG:HB2	1:A:87:ARG:NE	2.26	0.51
2:B:262:TYR:CD1	2:B:262:TYR:N	2.78	0.51
1:A:97:THR:HG22	1:A:221:LYS:HZ1	1.76	0.50
2:B:318:VAL:HG12	2:B:319:GLY:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:PHE:CZ	2:B:417:TYR:CD1	2.99	0.50
2:B:320:LEU:O	2:B:320:LEU:HD12	2.12	0.50
2:B:260:ASN:HD21	2:B:416:SER:CB	2.24	0.50
2:B:245:GLN:O	2:B:246:ASP:HB3	2.11	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:110:VAL:C	1:A:111:LEU:HD13	2.32	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
2:B:288:MET:HE2	2:B:292:ALA:CB	2.43	0.49
1:A:122:VAL:HG23	1:A:127:ARG:CA	2.40	0.49
1:A:72:ARG:HH12	1:A:171:THR:H	1.56	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:276:LEU:O	2:B:277:ARG:C	2.50	0.48
2:B:357:LYS:HG2	2:B:358:ALA:N	2.27	0.48
1:A:202:PRO:C	1:A:204:ASP:H	2.16	0.48
1:A:69:LEU:HA	1:A:89:LEU:HD12	1.95	0.48
2:B:322:GLN:NE2	2:B:324:GLN:CB	2.72	0.48
1:A:60:PHE:CE1	1:A:219:ILE:HD12	2.48	0.48
2:B:265:LEU:HG	2:B:285:CYS:O	2.13	0.48
1:A:176:PHE:N	1:A:176:PHE:CD1	2.82	0.48
1:A:148:LEU:HD12	1:A:149:ILE:N	2.29	0.48
1:A:196:GLU:HG2	1:A:202:PRO:HA	1.96	0.48
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
2:B:324:GLN:NE2	2:B:324:GLN:CA	2.77	0.48
1:A:103:HIS:HB2	1:A:144:THR:O	2.14	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
2:B:264:LYS:O	2:B:286:LEU:HD22	2.14	0.47
1:A:83:LEU:HD21	2:B:369:VAL:HG21	1.96	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:118:ILE:HA	1:A:131:LYS:HA	1.95	0.47
1:A:71:GLN:HA	1:A:87:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:LEU:CD1	2:B:329:GLU:N	2.78	0.47
1:A:76:ASP:N	1:A:76:ASP:OD1	2.48	0.47
2:B:306:LEU:HB3	2:B:346:ILE:CG2	2.44	0.47
1:A:222:MET:HB3	1:A:223:PRO:CD	2.45	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
1:A:54:ASN:N	1:A:54:ASN:OD1	2.48	0.47
2:B:257:ILE:CD1	2:B:258:TYR:CD2	2.99	0.46
2:B:262:TYR:C	2:B:289:ASN:ND2	2.63	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
2:B:257:ILE:CG1	2:B:258:TYR:CD2	2.98	0.46
1:A:44:ALA:HB3	1:A:71:GLN:NE2	2.30	0.46
1:A:82:ASN:C	1:A:84:ARG:H	2.18	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
1:A:117:ALA:C	1:A:132:LEU:H	2.17	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:422:GLN:HA	2:B:423:PRO:HD2	1.51	0.46
2:B:259:SER:HB3	2:B:264:LYS:HG2	1.97	0.45
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
2:B:390:ILE:HG22	2:B:391:PRO:HD2	1.98	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: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:206:ILE:O	1:A:210:LEU:HB2	2.16	0.45
2:B:306:LEU:HD22	2:B:348:ILE:HD12	1.98	0.45
1:A:196:GLU:OE2	1:A:202:PRO:HA	2.17	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
2:B:260:ASN:OD1	2:B:262:TYR:CD1	2.70	0.45
1:A:223:PRO:CD	1:A:224:LYS:N	2.79	0.45
1:A:224:LYS:HG3	1:A:224:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:CZ	1:A:79:LYS:CD	3.00	0.45
1:A:221:LYS:CA	1:A:221:LYS:NZ	2.74	0.45
2:B:286:LEU:C	2:B:287:GLN:CG	2.81	0.45
2:B:405:GLU:O	2:B:409:LEU:HD12	2.16	0.45
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: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
1:A:62:ASN:ND2	1:A:216:GLU:HB2	2.28	0.44
1:A:58:THR:O	1:A:58:THR:HG22	2.17	0.44
1:A:221:LYS:NZ	1:A:221:LYS:CB	2.76	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:129:THR:HB	2:B:242:LEU:HD13	1.99	0.44
1:A:208:GLN:C	1:A:209:THR:HG1	2.17	0.44
2:B:386:VAL:O	2:B:389:GLN:N	2.49	0.44
1:A:128:ASP:OD2	1:A:130:TYR:OH	2.24	0.44
1:A:110:VAL:HG12	1:A:159:ILE:CD1	2.47	0.44
1:A:52:ARG:HH21	1:A:54:ASN:ND2	2.16	0.44
2:B:303:THR:HG23	2:B:349:PRO:HA	2.00	0.43
2:B:253:SER:CB	2:B:266:TYR:CD2	2.98	0.43
1:A:111:LEU:N	1:A:111:LEU:HD13	2.33	0.43
1:A:100:LEU:HG	1:A:218:VAL:O	2.18	0.43
1:A:97:THR:HG22	1:A:221:LYS:NZ	2.32	0.43
1:A:118:ILE:HD13	1:A:131:LYS:HA	2.01	0.43
2:B:281:ILE:HA	2:B:368:GLY:O	2.18	0.43
1:A:183:LEU:HA	1:A:184:PRO:HD3	1.54	0.43
1:A:83:LEU:HD22	2:B:369:VAL:HG21	1.99	0.43
1:A:199:TYR:CD2	1:A:206:ILE:HG12	2.53	0.43
1:A:97:THR:HA	1:A:220:VAL:O	2.18	0.43
2:B:340:LEU:HD22	2:B:344:ASP:HB3	2.00	0.43
2:B:387:ILE:C	2:B:389:GLN:N	2.71	0.43
2:B:268:ILE:CG2	2:B:273:ASN:HB2	2.48	0.43
1:A:69:LEU:CD2	1:A:87:ARG:NH1	2.75	0.43
2:B:313:ALA:C	2:B:339:THR:HG23	2.39	0.43
2:B:420:ASP:CG	2:B:422:GLN:HB2	2.39	0.43
1:A:183:LEU:O	1:A:184:PRO:O	2.37	0.43
2:B:354:VAL:HG22	2:B:355:ALA:N	2.32	0.43
1:A:49:TYR:CZ	1:A:79:LYS:HD2	2.51	0.43
1:A:202:PRO:HB2	1:A:204:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:O	1:A:209:THR:N	2.51	0.43
2:B:286:LEU:O	2:B:287:GLN:HG2	2.19	0.43
1:A:102:HIS:HB3	1:A:176:PHE:HA	2.00	0.43
1:A:52:ARG:NH2	1:A:54:ASN:ND2	2.66	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:315:VAL:HG21	2:B:346:ILE:HD13	2.00	0.42
2:B:247:LYS:H	2:B:247:LYS:HG3	1.00	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
2:B:322:GLN:HE21	2:B:324:GLN:HB3	1.80	0.42
2:B:324:GLN:HE21	2:B:324:GLN:CA	2.32	0.42
1:A:207:GLU:OE2	1:A:211:LEU:CD2	2.67	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
2:B:273:ASN:OD1	2:B:274:SER:N	2.53	0.42
1:A:56:PHE:N	1:A:56:PHE:CD1	2.88	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
2:B:251:LEU:CD1	2:B:268:ILE:CD1	2.94	0.42
2:B:415:GLU:CB	2:B:419:VAL:CG2	2.97	0.42
1:A:155:GLN:HG2	1:A:156:ASN:ND2	2.35	0.42
1:A:117:ALA:HB2	1:A:157:LEU:CD1	2.49	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:CE2	1:A:218:VAL:HG23	2.54	0.42
1:A:110:VAL:HG13	1:A:159:ILE:CG2	2.41	0.42
1:A:85:ASP:HA	1:A:170:GLY:N	2.35	0.42
1:A:60:PHE:CD2	1:A:218:VAL:HB	2.55	0.42
2:B:403:GLY:O	2:B:407:GLU:HB2	2.19	0.42
1:A:222:MET:HE1	1:A:224:LYS:CE	2.49	0.42
2:B:257:ILE:HD12	2:B:258:TYR:HE2	1.76	0.42
1:A:108:LEU:HB2	1:A:140:ILE:O	2.20	0.42
2:B:293:LEU:O	2:B:418:PHE:HA	2.20	0.42
2:B:288:MET:HE1	2:B:293:LEU:CA	2.49	0.42
2:B:342:GLU:O	2:B:342:GLU:HG2	2.20	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:212:GLN:HB2	1:A:213:GLU:H	1.71	0.41
1:A:144:THR:CG2	1:A:145:PRO:N	2.82	0.41
1:A:141:GLN:O	1:A:142:ALA:O	2.37	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
1:A:176:PHE:CE2	1:A:218:VAL:CG1	3.03	0.41
2:B:268:ILE:O	2:B:283:LEU:N	2.47	0.41
1:A:83:LEU:HB3	1:A:86:TYR:CD2	2.55	0.41
2:B:288:MET:HE1	2:B:293:LEU:HA	2.03	0.41
1:A:63:GLN:O	1:A:64:HIS:CG	2.73	0.41
2:B:260:ASN:C	2:B:262:TYR:N	2.74	0.41
2:B:378:PHE:CD2	2:B:384:GLU:CB	2.98	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: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:245:GLN:HG2	2:B:245:GLN:H	1.71	0.41
1:A:169:PRO:C	1:A:171:THR:H	2.25	0.40
2:B:324:GLN:C	2:B:325:GLN:OE1	2.59	0.40
2:B:415:GLU:HB2	2:B:419:VAL:HG22	2.03	0.40
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:N	1:A:152:ASP:OD1	2.30	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:HA	1:A:70:LEU:HD12	1.90	0.40
2:B:396:ASP:CG	2:B:402:SER:OG	2.59	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 (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%)	126 (70%)	30 (17%)	23 (13%)	0	0
2	B	182/184 (99%)	130 (71%)	35 (19%)	17 (9%)	1	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

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Mol	Chain	Res	Type
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 (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%)	100 (60%)	67 (40%)	0 0
2	B	161/161 (100%)	87 (54%)	74 (46%)	0 0
All	All	328/328 (100%)	187 (57%)	141 (43%)	0 0

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	47	ASN
1	A	49	TYR
1	A	50	LEU
1	A	54	ASN
1	A	55	LYS
1	A	60	PHE
1	A	63	GLN

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Mol	Chain	Res	Type
1	A	67	LEU
1	A	76	ASP
1	A	81	GLU
1	A	82	ASN
1	A	83	LEU
1	A	84	ARG
1	A	85	ASP
1	A	88	VAL
1	A	89	LEU
1	A	94	LYS
1	A	97	THR
1	A	102	HIS
1	A	104	SER
1	A	109	LEU
1	A	111	LEU
1	A	112	VAL
1	A	120	VAL
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	188	SER

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Mol	Chain	Res	Type
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	221	LYS
1	A	222	MET
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	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	282	LEU
2	B	284	ASN
2	B	285	CYS
2	B	286	LEU

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Mol	Chain	Res	Type
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	301	ARG
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
2	B	325	GLN
2	B	328	LEU
2	B	330	SER
2	B	333	LEU
2	B	334	ARG
2	B	341	SER
2	B	345	ILE
2	B	347	VAL
2	B	351	SER
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	373	ASN
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	390	ILE
2	B	392	ARG

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Mol	Chain	Res	Type
2	B	393	GLN
2	B	395	SER
2	B	396	ASP
2	B	397	LEU
2	B	402	SER
2	B	414	LYS
2	B	419	VAL

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

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%)	-0.87	0	100	100	11, 25, 33, 37	0
2	B	184/184 (100%)	-0.84	0	100	100	11, 25, 35, 45	0
All	All	365/365 (100%)	-0.86	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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.