W O R L D W I D E

wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:40 PM GMT

PDB ID	:	3UJP
Title	:	Structure of MntC protein at 2.7A
Authors	:	Kanteev, M.; Adir, N.
Deposited on	:	2011-11-08
Resolution	:	2.70 Å(reported)

The following versions of software and data (see references (i)) 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 ⓘ

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

The reported resolution of this entry is 2.70 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.289
Clashscore		49
Ramachandran outliers		4.8%
Sidechain outliers		18.2%
RSRZ outliers		4.7%

Worse　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
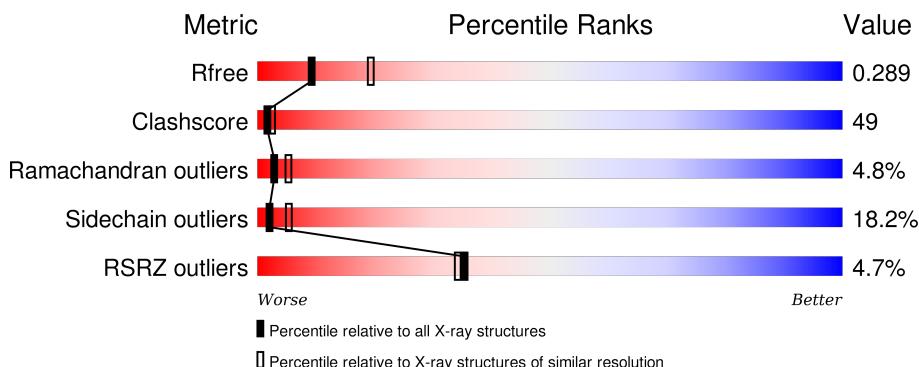
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	307	2% 39% 40% 10% 11%
1	B	307	4% 34% 40% 12% • 13%
1	C	307	7% 33% 39% 15% • 11%
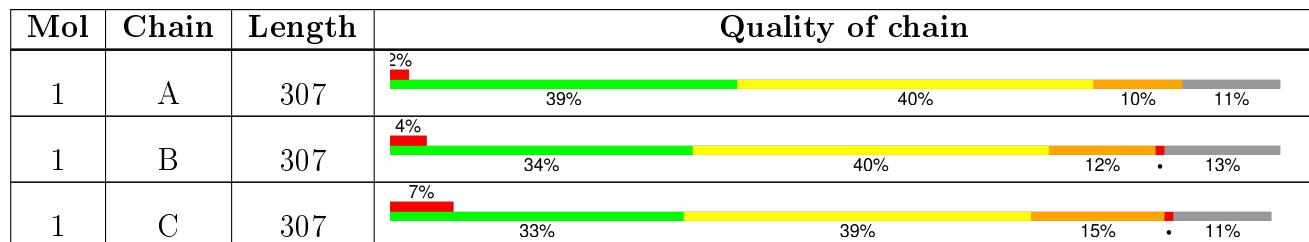
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	C	4	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6424 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 Mn transporter subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total 2149	C 1365	N 352	O 425	S 7	0	0	0
1	B	267	Total 2097	C 1333	N 345	O 412	S 7	0	0	0
1	C	272	Total 2137	C 1358	N 350	O 422	S 7	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	Zn 4	0	0
3	C	2	Total 2	Zn 2	0	0

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).
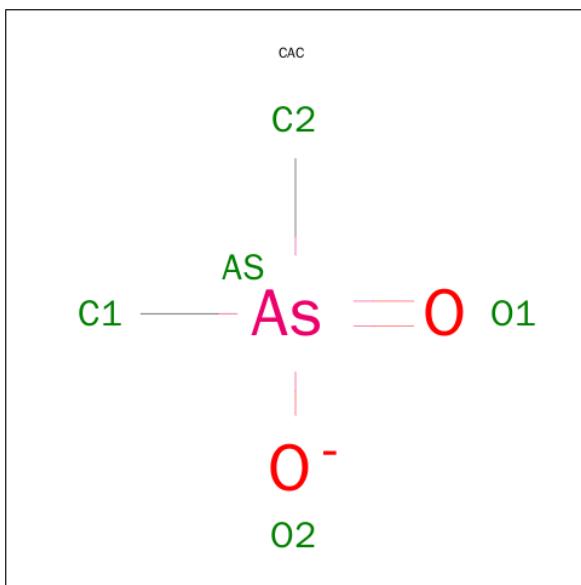
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total As C O 5 1 2 2			0	0
4	A	1	Total As C O 5 1 2 2			0	0
4	C	1	Total As C O 5 1 2 2			0	0
4	C	1	Total As C O 5 1 2 2			0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total O 6 6		0	0
5	B	5	Total O 5 5		0	0
5	C	1	Total O 1 1		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: Mn transporter subunit

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Chain C:
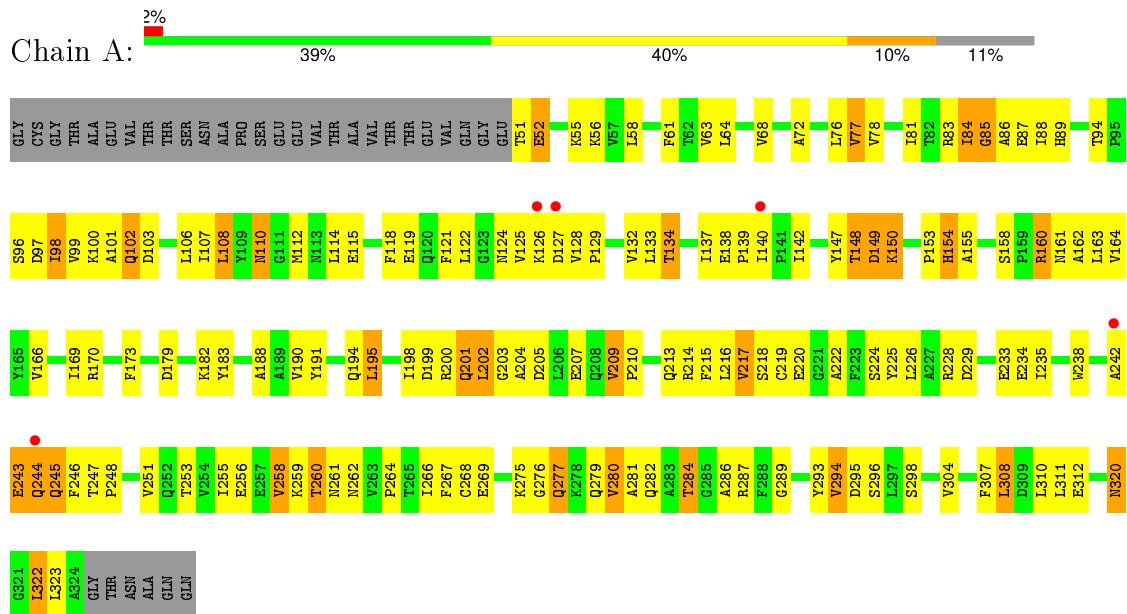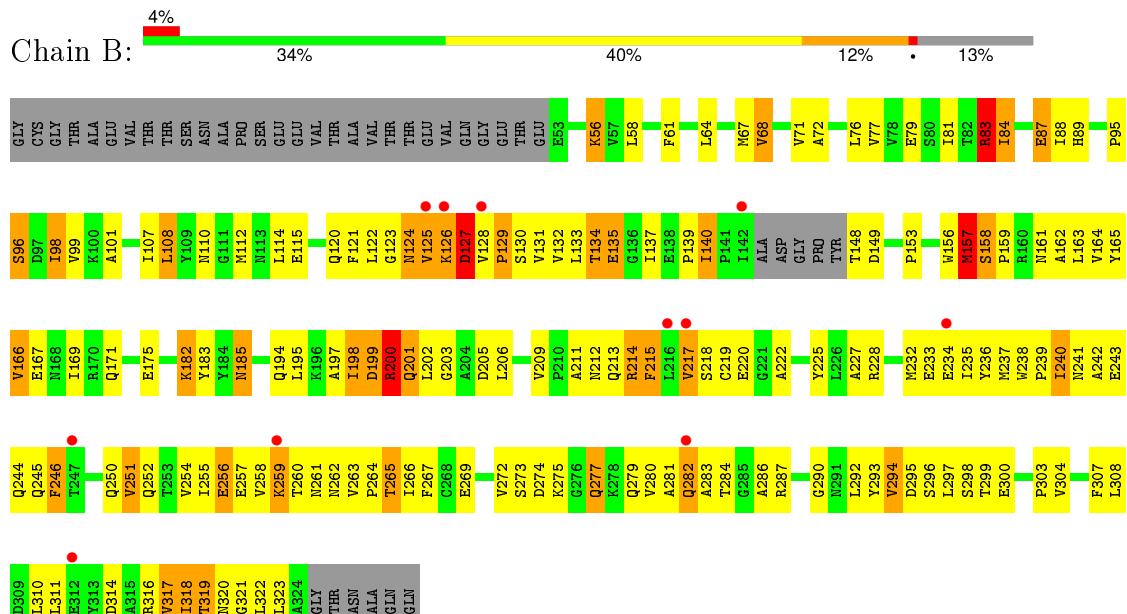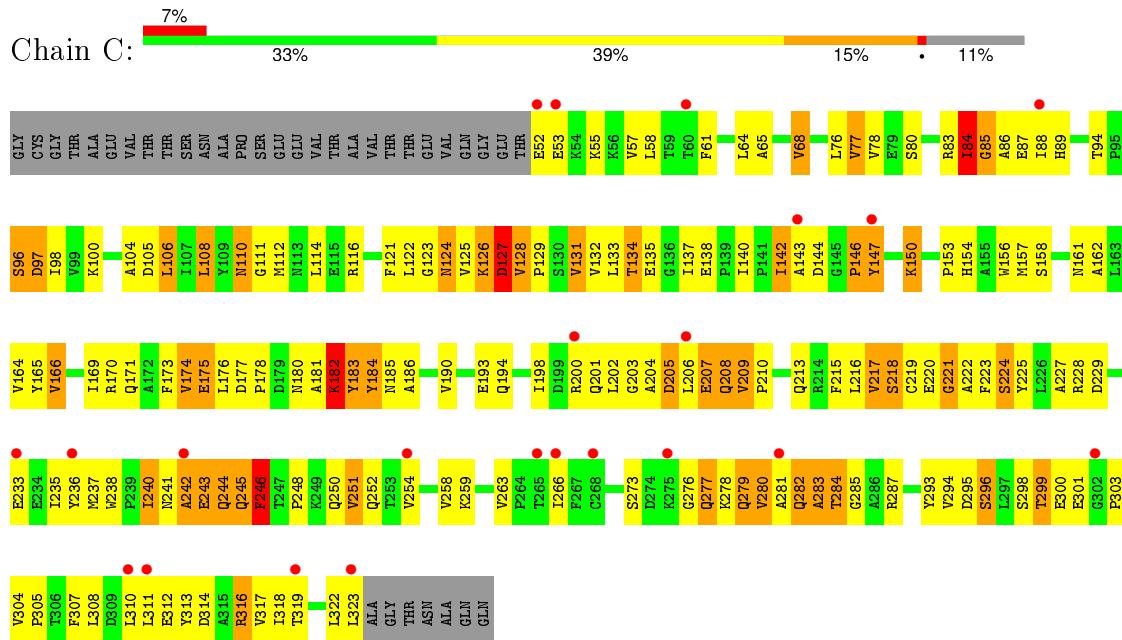
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.52Å 127.52Å 89.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.80 – 2.70 69.64 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.0 (36.80-2.70) 92.0 (69.64-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.231 , 0.284 0.237 , 0.289	Depositor DCC
R_{free} test set	2056 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	83.7	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 64.5	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Outliers	1 of 21603 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6424	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN, MN

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	0.60	0/2194	0.74	0/2991
1	B	0.66	1/2139 (0.0%)	0.73	0/2913
1	C	0.56	0/2182	0.67	0/2974
All	All	0.61	1/6515 (0.0%)	0.71	0/8878

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	GLY	C-N	-5.13	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2149	0	2097	164	0
1	B	2097	0	2055	242	0
1	C	2137	0	2087	231	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
4	A	10	0	0	4	0
4	C	10	0	0	0	0
5	A	6	0	0	0	0
5	B	5	0	0	2	0
5	C	1	0	0	0	0
All	All	6424	0	6239	622	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 49.

All (622) 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:B:213:GLN:HA	1:B:215:PHE:CE1	1.42	1.52
1:B:213:GLN:CA	1:B:215:PHE:HE1	1.44	1.28
1:B:258:VAL:HG22	1:B:263:VAL:CG2	1.68	1.22
1:B:265:THR:HB	1:B:321:GLY:O	1.41	1.20
1:C:89:HIS:CD2	1:C:295:ASP:OD2	1.98	1.17
1:B:127:ASP:O	1:B:128:VAL:HG23	1.45	1.15
1:C:203:GLY:O	1:C:207:GLU:HG2	1.42	1.15
1:C:259:LYS:HG2	1:C:284:THR:OG1	1.45	1.14
1:B:257:GLU:HA	1:B:260:THR:CG2	1.78	1.13
1:B:257:GLU:HA	1:B:260:THR:HG22	1.11	1.11
1:C:154:HIS:CG	1:C:222:ALA:HB1	1.85	1.10
1:B:219:CYS:HB3	1:B:238:TRP:CH2	1.86	1.08
1:B:238:TRP:CE2	1:B:244:GLN:NE2	2.21	1.06
1:B:258:VAL:HA	1:B:263:VAL:HG22	1.34	1.03
1:B:314:ASP:O	1:B:318:ILE:HG13	1.57	1.03
1:C:220:GLU:O	1:C:220:GLU:HG2	1.51	1.03
1:B:255:ILE:CG2	1:B:280:VAL:HA	1.88	1.02
1:C:248:PRO:HA	1:C:251:VAL:HG13	1.41	1.02
1:C:127:ASP:O	1:C:128:VAL:HG13	1.59	1.01
1:C:170:ARG:O	1:C:174:VAL:HG13	1.60	1.01
1:A:148:THR:HG22	1:A:149:ASP:N	1.72	1.01
1:B:238:TRP:CD2	1:B:244:GLN:NE2	2.29	1.00
1:B:257:GLU:CA	1:B:260:THR:HG22	1.91	1.00
1:B:240:ILE:HG23	1:B:241:ASN:O	1.63	0.99
1:C:277:GLN:HA	1:C:277:GLN:HE21	1.25	0.98
1:C:278:LYS:O	1:C:281:ALA:HB3	1.64	0.98
1:C:284:THR:HG22	1:C:284:THR:O	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ALA:O	1:C:282:GLN:HG3	1.63	0.97
1:B:263:VAL:O	1:B:263:VAL:HG23	1.63	0.97
1:A:258:VAL:HG12	1:A:259:LYS:N	1.78	0.96
1:B:125:VAL:O	1:B:125:VAL:HG22	1.63	0.96
1:C:142:ILE:HG22	1:C:143:ALA:H	1.31	0.96
1:B:126:LYS:HE3	1:C:84:ILE:HD13	1.48	0.95
1:A:148:THR:CG2	1:A:149:ASP:N	2.30	0.95
1:A:112:MET:CE	1:A:139:PRO:HB3	1.97	0.94
1:B:238:TRP:CD1	1:B:244:GLN:NE2	2.36	0.93
1:A:137:ILE:HG12	1:A:164:VAL:HG21	1.48	0.93
1:B:213:GLN:CA	1:B:215:PHE:CE1	2.30	0.92
1:C:219:CYS:HB3	1:C:238:TRP:CZ2	2.04	0.92
1:A:112:MET:HG3	1:A:134:THR:HG21	1.48	0.92
1:C:219:CYS:HB3	1:C:238:TRP:CH2	2.05	0.92
1:A:126:LYS:HG2	1:A:127:ASP:H	1.32	0.92
1:B:255:ILE:HG22	1:B:280:VAL:HA	1.53	0.91
1:C:154:HIS:CD2	1:C:222:ALA:HB1	2.06	0.91
1:A:242:ALA:O	1:A:243:GLU:HG2	1.72	0.90
1:B:238:TRP:CG	1:B:244:GLN:NE2	2.41	0.89
1:C:259:LYS:HG2	1:C:284:THR:HG1	1.37	0.89
1:A:242:ALA:O	1:A:243:GLU:CG	2.21	0.88
1:C:266:ILE:HD13	1:C:280:VAL:HG12	1.56	0.87
1:C:137:ILE:HG12	1:C:164:VAL:HG21	1.57	0.87
1:A:255:ILE:HG13	1:A:280:VAL:HB	1.56	0.87
1:B:137:ILE:HD11	1:B:164:VAL:CG2	2.03	0.86
1:B:319:THR:O	1:B:323:LEU:HD13	1.74	0.86
1:A:154:HIS:HE1	1:A:220:GLU:OE2	1.58	0.86
1:B:265:THR:HG21	1:B:267:PHE:CZ	2.11	0.85
1:A:203:GLY:HA3	1:C:301:GLU:OE2	1.76	0.85
1:C:175:GLU:HG2	1:C:176:LEU:N	1.91	0.85
1:A:284:THR:HG22	1:A:286:ALA:H	1.40	0.85
1:B:251:VAL:O	1:B:255:ILE:HG13	1.77	0.84
1:A:242:ALA:C	1:A:243:GLU:HG2	1.97	0.84
1:B:265:THR:CG2	1:B:267:PHE:CZ	2.61	0.84
1:B:298:SER:HB3	1:B:303:PRO:O	1.77	0.84
1:C:220:GLU:HB2	1:C:241:ASN:OD1	1.77	0.84
1:B:185:ASN:N	1:B:185:ASN:HD22	1.72	0.84
1:B:238:TRP:NE1	1:B:244:GLN:NE2	2.26	0.83
1:B:137:ILE:HD11	1:B:164:VAL:HG23	1.61	0.83
1:C:125:VAL:O	1:C:127:ASP:N	2.12	0.83
1:A:154:HIS:O	1:A:225:TYR:CD2	2.30	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:HD12	1:A:124:ASN:HD21	1.43	0.83
1:A:264:PRO:HG2	1:A:322:LEU:HA	1.61	0.83
1:C:175:GLU:O	1:C:178:PRO:HD3	1.80	0.82
1:B:258:VAL:HG22	1:B:263:VAL:HG21	1.61	0.81
1:A:280:VAL:O	1:A:284:THR:HB	1.79	0.81
1:B:258:VAL:CA	1:B:263:VAL:HG22	2.11	0.81
1:A:142:ILE:HG13	1:A:150:LYS:O	1.79	0.80
1:B:258:VAL:HG22	1:B:263:VAL:HG22	1.64	0.80
1:C:283:ALA:O	1:C:284:THR:HB	1.82	0.80
1:C:284:THR:CG2	1:C:284:THR:O	2.30	0.80
1:B:240:ILE:CG2	1:B:241:ASN:O	2.30	0.80
1:C:147:TYR:HB3	1:C:150:LYS:HG3	1.63	0.80
1:C:96:SER:O	1:C:100:LYS:HG2	1.82	0.80
1:A:55:LYS:HB2	1:A:76:LEU:HD22	1.64	0.80
1:C:278:LYS:O	1:C:281:ALA:CB	2.30	0.79
1:B:237:MET:HG3	1:B:254:VAL:HG21	1.64	0.79
1:B:277:GLN:HE21	1:B:277:GLN:HA	1.45	0.79
1:B:125:VAL:O	1:B:125:VAL:CG2	2.30	0.79
1:A:258:VAL:CG1	1:A:259:LYS:N	2.45	0.79
1:C:217:VAL:CG2	1:C:217:VAL:O	2.30	0.79
1:A:96:SER:O	1:A:99:VAL:HG12	1.82	0.78
1:C:246:PHE:CE2	1:C:276:GLY:HA3	2.19	0.78
1:B:110:ASN:O	1:B:134:THR:HB	1.83	0.78
1:B:128:VAL:HG12	1:B:128:VAL:O	1.81	0.78
1:B:126:LYS:HE3	1:C:84:ILE:CD1	2.13	0.78
1:B:256:GLU:OE1	1:B:260:THR:HG21	1.84	0.78
1:C:157:MET:SD	1:C:294:VAL:HG12	2.24	0.78
1:C:125:VAL:O	1:C:126:LYS:C	2.23	0.77
1:A:217:VAL:HG11	1:A:266:ILE:HG22	1.65	0.77
1:B:209:VAL:CG2	1:B:213:GLN:O	2.33	0.77
1:B:258:VAL:HG22	1:B:263:VAL:HG23	1.66	0.76
1:C:298:SER:HB3	1:C:303:PRO:O	1.85	0.76
1:B:194:GLN:O	1:B:198:ILE:HG23	1.85	0.76
1:A:148:THR:HG22	1:A:149:ASP:H	1.47	0.76
1:B:137:ILE:N	1:B:137:ILE:HD12	2.00	0.76
1:B:127:ASP:O	1:B:128:VAL:CG2	2.30	0.76
1:B:198:ILE:HD11	1:B:311:LEU:HD13	1.67	0.76
1:C:65:ALA:HB2	1:C:80:SER:HB2	1.66	0.76
1:C:278:LYS:O	1:C:281:ALA:CA	2.33	0.76
1:B:185:ASN:ND2	1:B:185:ASN:N	2.31	0.76
1:A:154:HIS:CE1	1:A:220:GLU:OE2	2.39	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:CG2	1:B:263:VAL:CG2	2.59	0.75
1:C:125:VAL:HB	1:C:128:VAL:CG2	2.16	0.75
1:B:258:VAL:HG11	1:B:286:ALA:HB2	1.69	0.74
1:B:107:ILE:CD1	1:B:128:VAL:HG11	2.17	0.74
1:C:206:LEU:HD23	1:C:319:THR:OG1	1.86	0.74
1:A:110:ASN:O	1:A:134:THR:HB	1.87	0.73
1:A:154:HIS:O	1:A:225:TYR:HD2	1.68	0.73
1:C:281:ALA:O	1:C:282:GLN:CG	2.34	0.73
1:B:263:VAL:O	1:B:263:VAL:CG2	2.35	0.73
1:B:215:PHE:N	1:B:215:PHE:CD1	2.55	0.72
1:B:280:VAL:O	1:B:284:THR:HG22	1.89	0.72
1:C:122:LEU:O	1:C:125:VAL:HG22	1.89	0.71
1:B:126:LYS:HG2	1:C:299:THR:HG23	1.72	0.71
1:A:84:ILE:HG23	1:A:85:GLY:N	2.03	0.71
1:C:98:ILE:HD13	1:C:124:ASN:HD22	1.55	0.71
1:C:165:TYR:O	1:C:169:ILE:HG13	1.91	0.70
1:A:154:HIS:ND1	1:A:222:ALA:HA	2.06	0.70
1:C:64:LEU:O	1:C:68:VAL:HG13	1.91	0.70
1:B:200:ARG:O	1:B:203:GLY:N	2.22	0.70
1:C:108:LEU:HD12	1:C:131:VAL:HG13	1.73	0.70
1:A:88:ILE:HG12	1:A:295:ASP:HB3	1.73	0.70
1:B:107:ILE:HD11	1:B:128:VAL:HG11	1.74	0.70
1:B:83:ARG:NE	1:B:83:ARG:HA	2.06	0.70
1:A:112:MET:HE1	1:A:139:PRO:HB3	1.73	0.70
1:A:242:ALA:O	1:A:243:GLU:CB	2.39	0.70
1:B:159:PRO:CB	1:B:199:ASP:HB2	2.22	0.70
1:B:107:ILE:HD12	1:B:128:VAL:CG1	2.22	0.70
1:C:216:LEU:HD11	1:C:318:ILE:HD13	1.74	0.69
1:C:217:VAL:HG21	1:C:266:ILE:HG22	1.74	0.69
1:C:254:VAL:O	1:C:258:VAL:HG12	1.92	0.69
1:A:51:THR:O	1:A:51:THR:HG23	1.91	0.69
1:B:258:VAL:O	1:B:262:ASN:HA	1.93	0.69
1:C:147:TYR:CB	1:C:150:LYS:HG3	2.23	0.69
1:C:183:TYR:O	1:C:186:ALA:N	2.25	0.69
1:A:218:SER:HA	1:A:267:PHE:O	1.93	0.69
1:C:127:ASP:C	1:C:128:VAL:HG22	2.14	0.68
1:C:106:LEU:HD11	1:C:131:VAL:HG12	1.75	0.68
1:C:246:PHE:HE2	1:C:276:GLY:HA3	1.56	0.68
1:A:200:ARG:HA	1:C:301:GLU:OE1	1.94	0.68
1:C:217:VAL:HA	1:C:235:ILE:O	1.93	0.68
1:B:137:ILE:CD1	1:B:164:VAL:HG21	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LYS:HB2	1:C:76:LEU:HD22	1.76	0.68
1:A:126:LYS:HG2	1:A:127:ASP:N	2.07	0.68
1:C:154:HIS:CD2	1:C:222:ALA:CB	2.76	0.68
1:B:96:SER:O	1:B:99:VAL:HG12	1.94	0.68
1:B:162:ALA:O	1:B:166:VAL:HG13	1.94	0.68
1:B:83:ARG:HE	1:B:83:ARG:HA	1.59	0.67
1:A:161:ASN:O	1:A:164:VAL:HG22	1.95	0.67
1:A:98:ILE:CD1	1:A:124:ASN:HD21	2.06	0.67
1:A:275:LYS:O	1:A:279:GLN:HG3	1.93	0.67
1:B:132:VAL:HG23	1:B:134:THR:H	1.58	0.67
1:A:201:GLN:O	1:A:201:GLN:HG3	1.94	0.67
1:C:278:LYS:O	1:C:281:ALA:C	2.34	0.67
1:C:266:ILE:HD13	1:C:280:VAL:CG1	2.24	0.67
1:B:114:LEU:HB2	1:B:153:PRO:HB2	1.77	0.66
1:B:240:ILE:HG22	1:B:240:ILE:O	1.95	0.66
1:C:278:LYS:HA	1:C:281:ALA:HB3	1.78	0.66
1:B:185:ASN:ND2	1:B:185:ASN:H	1.92	0.66
1:B:64:LEU:HD13	1:B:133:LEU:HD12	1.78	0.66
1:C:279:GLN:C	1:C:281:ALA:N	2.48	0.66
1:C:224:SER:O	1:C:227:ALA:HB3	1.96	0.66
1:C:218:SER:OG	1:C:219:CYS:N	2.28	0.65
1:B:137:ILE:HD11	1:B:164:VAL:HG21	1.74	0.65
1:B:198:ILE:HD12	1:B:198:ILE:O	1.96	0.65
1:B:122:LEU:HA	1:B:125:VAL:CG1	2.26	0.65
1:C:279:GLN:O	1:C:282:GLN:N	2.30	0.65
1:C:220:GLU:O	1:C:222:ALA:N	2.30	0.65
1:C:154:HIS:CG	1:C:222:ALA:CB	2.74	0.65
1:A:108:LEU:HG	1:A:133:LEU:HD21	1.77	0.65
1:C:142:ILE:HG22	1:C:143:ALA:N	2.08	0.65
1:C:278:LYS:O	1:C:281:ALA:N	2.30	0.65
1:A:153:PRO:O	1:A:155:ALA:N	2.30	0.65
1:C:248:PRO:HA	1:C:251:VAL:CG1	2.22	0.65
1:C:180:ASN:HB2	1:C:184:TYR:CE2	2.31	0.65
1:B:251:VAL:O	1:B:255:ILE:CG1	2.45	0.64
1:C:220:GLU:CG	1:C:220:GLU:O	2.36	0.64
1:C:173:PHE:O	1:C:175:GLU:N	2.30	0.64
1:C:279:GLN:O	1:C:281:ALA:N	2.30	0.64
1:A:277:GLN:HA	1:A:277:GLN:HE21	1.62	0.64
1:C:244:GLN:C	1:C:245:GLN:HG2	2.18	0.64
1:A:98:ILE:HG21	1:A:124:ASN:ND2	2.13	0.64
1:B:265:THR:CB	1:B:321:GLY:O	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PHE:CE2	1:B:64:LEU:HG	2.32	0.64
1:C:142:ILE:HG13	1:C:150:LYS:O	1.97	0.63
1:B:182:LYS:HG2	1:B:183:TYR:N	2.12	0.63
1:C:307:PHE:CZ	1:C:311:LEU:HD11	2.33	0.63
1:B:213:GLN:HA	1:B:215:PHE:HE1	0.55	0.63
1:B:257:GLU:OE1	1:B:261:ASN:ND2	2.32	0.63
1:A:58:LEU:HD23	1:A:81:ILE:HD11	1.79	0.63
1:C:147:TYR:N	1:C:147:TYR:CD1	2.64	0.63
1:A:126:LYS:CG	1:A:127:ASP:H	2.09	0.63
1:B:72:ALA:HB1	1:B:76:LEU:HB2	1.80	0.63
1:B:58:LEU:HD21	1:B:81:ILE:HD11	1.81	0.63
1:B:209:VAL:HG22	1:B:213:GLN:O	1.97	0.62
1:B:107:ILE:CD1	1:B:128:VAL:CG1	2.77	0.62
1:B:255:ILE:HG22	1:B:280:VAL:CA	2.27	0.62
1:B:107:ILE:HD12	1:B:128:VAL:HG12	1.81	0.62
1:C:124:ASN:N	1:C:124:ASN:OD1	2.31	0.62
1:A:312:GLU:OE2	4:A:332:CAC:C1	2.47	0.62
1:B:255:ILE:HG23	1:B:280:VAL:HB	1.80	0.62
1:A:84:ILE:O	1:A:86:ALA:N	2.33	0.62
1:C:125:VAL:HB	1:C:128:VAL:HG21	1.82	0.62
1:C:217:VAL:HG23	1:C:217:VAL:O	1.99	0.62
1:B:126:LYS:O	1:B:127:ASP:C	2.36	0.62
1:C:240:ILE:HG23	1:C:241:ASN:O	2.00	0.62
1:B:255:ILE:CG2	1:B:280:VAL:CA	2.72	0.62
1:C:137:ILE:CG1	1:C:164:VAL:HG21	2.29	0.62
1:B:304:VAL:HG13	1:B:310:LEU:HB2	1.82	0.62
1:B:258:VAL:CG2	1:B:263:VAL:HG22	2.28	0.61
1:B:122:LEU:HA	1:B:125:VAL:HG13	1.81	0.61
1:B:64:LEU:O	1:B:68:VAL:HG13	2.01	0.61
1:A:218:SER:HB2	1:A:269:GLU:OE2	2.01	0.61
1:C:278:LYS:C	1:C:281:ALA:HB3	2.20	0.61
1:A:215:PHE:CD2	1:A:233:GLU:HB3	2.36	0.61
1:B:212:ASN:O	1:B:215:PHE:CZ	2.54	0.61
1:C:203:GLY:O	1:C:207:GLU:CG	2.34	0.61
1:B:128:VAL:O	1:B:129:PRO:C	2.39	0.60
1:C:217:VAL:HG22	1:C:217:VAL:O	2.00	0.60
1:B:256:GLU:HG3	1:B:257:GLU:N	2.15	0.60
1:C:126:LYS:O	1:C:128:VAL:N	2.30	0.60
1:B:304:VAL:HG13	1:B:310:LEU:HA	1.82	0.60
1:B:198:ILE:HD12	1:B:198:ILE:C	2.23	0.60
1:B:265:THR:HG22	1:B:267:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:THR:HG23	1:B:261:ASN:ND2	2.17	0.59
1:C:200:ARG:HB3	1:C:200:ARG:NH2	2.17	0.59
1:C:243:GLU:HG2	1:C:244:GLN:N	2.16	0.59
1:A:158:SER:O	1:A:161:ASN:HB2	2.02	0.59
1:B:200:ARG:O	1:B:202:LEU:N	2.36	0.59
1:B:255:ILE:O	1:B:259:LYS:HE3	2.01	0.59
1:C:127:ASP:O	1:C:128:VAL:CG1	2.42	0.59
1:A:126:LYS:O	1:A:127:ASP:C	2.39	0.59
1:A:98:ILE:HD12	1:A:124:ASN:ND2	2.17	0.59
1:B:252:GLN:HA	1:B:255:ILE:HD11	1.85	0.59
1:C:277:GLN:HA	1:C:277:GLN:NE2	2.06	0.58
1:B:87:GLU:HG3	1:B:87:GLU:O	2.03	0.58
1:A:162:ALA:O	1:A:166:VAL:HG13	2.03	0.58
1:C:278:LYS:CA	1:C:281:ALA:HB3	2.32	0.58
1:A:198:ILE:C	1:A:198:ILE:HD12	2.24	0.58
1:B:233:GLU:HG3	1:B:234:GLU:N	2.19	0.58
1:B:148:THR:HG23	1:B:149:ASP:H	1.67	0.58
1:A:258:VAL:O	1:A:262:ASN:N	2.37	0.58
1:A:267:PHE:CE2	1:A:289:GLY:HA3	2.39	0.58
1:C:84:ILE:O	1:C:86:ALA:N	2.36	0.58
1:A:217:VAL:HG13	1:A:266:ILE:HA	1.86	0.58
1:C:217:VAL:HG21	1:C:266:ILE:CG2	2.33	0.57
1:C:68:VAL:HG12	1:C:169:ILE:HD13	1.86	0.57
1:A:160:ARG:HG3	1:A:229:ASP:OD2	2.04	0.57
1:C:116:ARG:NH2	1:C:242:ALA:HA	2.19	0.57
1:B:121:PHE:O	1:B:125:VAL:HG12	2.04	0.57
1:B:258:VAL:CB	1:B:263:VAL:HG22	2.35	0.57
1:A:98:ILE:CG2	1:A:124:ASN:ND2	2.67	0.57
1:B:212:ASN:O	1:B:215:PHE:HZ	1.88	0.57
1:B:95:PRO:HA	1:B:98:ILE:HG13	1.87	0.57
1:C:215:PHE:HD2	1:C:233:GLU:HB3	1.69	0.57
1:A:304:VAL:HG13	1:A:310:LEU:HA	1.86	0.57
1:B:137:ILE:N	1:B:137:ILE:CD1	2.67	0.57
1:C:201:GLN:NE2	1:C:312:GLU:HG3	2.19	0.57
1:B:161:ASN:O	1:B:164:VAL:HG22	2.05	0.56
1:B:293:TYR:CD1	1:B:304:VAL:HG21	2.39	0.56
1:C:220:GLU:O	1:C:221:GLY:C	2.42	0.56
1:C:182:LYS:O	1:C:185:ASN:HB2	2.06	0.56
1:C:246:PHE:HD1	1:C:246:PHE:O	1.88	0.56
1:C:266:ILE:HD12	1:C:277:GLN:HG3	1.88	0.56
1:B:134:THR:O	1:B:137:ILE:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASP:O	1:B:318:ILE:CG1	2.43	0.56
1:B:126:LYS:HG2	1:C:299:THR:CG2	2.36	0.56
1:A:261:ASN:O	1:A:262:ASN:C	2.42	0.56
1:C:61:PHE:CE2	1:C:64:LEU:HG	2.41	0.56
1:A:154:HIS:CE1	1:A:220:GLU:CD	2.79	0.55
1:A:255:ILE:CG1	1:A:280:VAL:HB	2.34	0.55
1:C:215:PHE:CD2	1:C:233:GLU:HB3	2.41	0.55
1:B:238:TRP:HZ2	1:B:272:VAL:HG21	1.71	0.55
1:B:107:ILE:HD12	1:B:128:VAL:HG11	1.87	0.55
1:C:143:ALA:HB2	1:C:236:TYR:OH	2.06	0.55
1:C:98:ILE:HD13	1:C:124:ASN:ND2	2.18	0.55
1:B:250:GLN:O	1:B:254:VAL:HG23	2.06	0.55
1:C:299:THR:HG22	1:C:300:GLU:H	1.71	0.55
1:C:84:ILE:HG23	1:C:85:GLY:N	2.20	0.55
1:A:106:LEU:HD13	1:A:129:PRO:HB2	1.88	0.55
1:B:56:LYS:HG3	1:B:77:VAL:HG13	1.88	0.55
1:A:260:THR:HG22	1:A:261:ASN:OD1	2.07	0.55
1:B:304:VAL:HG13	1:B:310:LEU:CB	2.37	0.55
1:B:244:GLN:O	1:B:245:GLN:HB2	2.06	0.55
1:B:220:GLU:OE2	1:B:241:ASN:OD1	2.25	0.55
1:A:203:GLY:CA	1:C:301:GLU:OE2	2.51	0.55
1:A:198:ILE:HA	1:A:201:GLN:HB3	1.89	0.55
1:A:61:PHE:CE1	1:A:63:VAL:HB	2.42	0.55
1:B:84:ILE:O	1:B:84:ILE:HG22	2.07	0.54
1:B:159:PRO:HB3	1:B:199:ASP:HB2	1.88	0.54
1:A:163:LEU:O	1:A:166:VAL:HG22	2.07	0.54
1:B:137:ILE:CG1	1:B:164:VAL:HG21	2.37	0.54
1:B:137:ILE:HG13	1:B:164:VAL:HG21	1.88	0.54
1:C:201:GLN:NE2	1:C:312:GLU:OE2	2.24	0.54
1:B:206:LEU:O	1:B:209:VAL:HG13	2.06	0.54
1:C:161:ASN:HD22	1:C:161:ASN:N	2.05	0.54
1:C:84:ILE:CG2	1:C:85:GLY:N	2.69	0.54
1:C:68:VAL:HG23	1:C:78:VAL:HG21	1.90	0.54
1:A:163:LEU:HD21	1:A:195:LEU:HB3	1.90	0.54
1:C:125:VAL:O	1:C:128:VAL:HG22	2.07	0.54
1:C:183:TYR:O	1:C:185:ASN:N	2.41	0.54
1:B:265:THR:HG21	1:B:267:PHE:HZ	1.69	0.54
1:C:106:LEU:HD22	1:C:176:LEU:HD22	1.90	0.54
1:C:98:ILE:CG1	1:C:121:PHE:CE1	2.90	0.54
1:A:248:PRO:HA	1:A:251:VAL:HG13	1.89	0.54
1:A:114:LEU:HD13	1:A:153:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ALA:HB2	1:A:173:PHE:CE2	2.43	0.54
1:A:72:ALA:HB2	1:A:173:PHE:HE2	1.72	0.54
1:B:213:GLN:HA	1:B:215:PHE:CD1	2.27	0.54
1:C:83:ARG:O	1:C:84:ILE:O	2.26	0.54
1:C:220:GLU:HG3	1:C:240:ILE:HA	1.90	0.54
1:B:227:ALA:HA	1:B:232:MET:HB2	1.90	0.54
1:C:125:VAL:O	1:C:127:ASP:CA	2.56	0.53
1:C:98:ILE:HG13	1:C:121:PHE:CE1	2.42	0.53
1:A:142:ILE:HB	1:A:148:THR:O	2.07	0.53
1:A:255:ILE:HD11	1:A:280:VAL:HA	1.90	0.53
1:B:304:VAL:HG13	1:B:310:LEU:CA	2.37	0.53
1:A:106:LEU:HD12	1:A:107:ILE:H	1.73	0.53
1:B:124:ASN:HA	1:C:84:ILE:HG21	1.90	0.53
1:B:282:GLN:HG3	1:B:283:ALA:N	2.23	0.53
1:B:167:GLU:OE1	1:B:167:GLU:HA	2.08	0.53
1:A:194:GLN:NE2	1:B:135:GLU:HA	2.23	0.53
1:C:209:VAL:HG12	1:C:323:LEU:CD1	2.38	0.53
1:C:209:VAL:HG12	1:C:323:LEU:HD11	1.89	0.53
1:C:140:ILE:HD11	1:C:228:ARG:HH21	1.72	0.53
1:B:218:SER:HB2	1:B:269:GLU:OE2	2.08	0.53
1:B:319:THR:HG22	1:B:320:ASN:N	2.22	0.53
1:B:220:GLU:CD	1:B:241:ASN:OD1	2.47	0.53
1:A:158:SER:HB2	1:A:225:TYR:HB3	1.91	0.53
1:C:314:ASP:O	1:C:318:ILE:HG13	2.07	0.53
1:B:235:ILE:HG12	1:B:257:GLU:HG3	1.91	0.53
1:C:201:GLN:HE22	1:C:312:GLU:CD	2.09	0.53
1:B:260:THR:HG23	1:B:261:ASN:HD22	1.73	0.53
1:B:67:MET:HE1	1:B:165:TYR:HB3	1.90	0.52
1:A:98:ILE:CG2	1:A:124:ASN:HD21	2.20	0.52
1:A:280:VAL:O	1:A:280:VAL:HG23	2.09	0.52
1:C:133:LEU:HD22	1:C:169:ILE:HG12	1.91	0.52
1:B:307:PHE:O	1:B:310:LEU:HB3	2.09	0.52
1:A:182:LYS:HE3	1:A:183:TYR:CE1	2.45	0.52
1:B:84:ILE:O	1:B:84:ILE:CG2	2.58	0.52
1:C:88:ILE:HD13	1:C:114:LEU:HD21	1.92	0.52
1:C:98:ILE:HG13	1:C:121:PHE:HE1	1.75	0.52
1:B:215:PHE:HD1	1:B:215:PHE:H	1.56	0.52
1:C:104:ALA:O	1:C:128:VAL:CG1	2.58	0.52
1:A:209:VAL:HG22	1:A:214:ARG:HG3	1.91	0.51
1:B:126:LYS:O	1:B:127:ASP:O	2.28	0.51
1:B:88:ILE:HG13	1:B:89:HIS:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:O	1:A:102:GLN:HG2	2.10	0.51
1:C:162:ALA:O	1:C:166:VAL:HG13	2.09	0.51
1:A:154:HIS:HE1	1:A:220:GLU:CD	2.14	0.51
1:B:159:PRO:HB2	1:B:199:ASP:HB2	1.92	0.51
1:A:244:GLN:O	1:A:245:GLN:C	2.47	0.51
1:B:258:VAL:HG13	1:B:263:VAL:O	2.11	0.51
1:C:313:TYR:O	1:C:314:ASP:C	2.48	0.51
1:A:204:ALA:HA	1:A:207:GLU:OE1	2.10	0.51
1:C:106:LEU:HD11	1:C:131:VAL:CG1	2.39	0.51
1:A:259:LYS:C	1:A:261:ASN:N	2.62	0.51
1:C:104:ALA:O	1:C:128:VAL:HG12	2.11	0.51
1:C:279:GLN:O	1:C:282:GLN:HB2	2.10	0.51
1:A:219:CYS:HB3	1:A:238:TRP:CH2	2.46	0.51
1:C:254:VAL:CG1	1:C:280:VAL:HG21	2.41	0.51
1:C:110:ASN:O	1:C:134:THR:HB	2.10	0.51
1:A:200:ARG:HG3	1:C:301:GLU:HB3	1.93	0.51
1:A:125:VAL:O	1:A:125:VAL:HG23	2.11	0.51
1:B:254:VAL:C	1:B:256:GLU:H	2.14	0.50
1:A:142:ILE:O	1:A:148:THR:O	2.29	0.50
1:C:223:PHE:CE2	1:C:294:VAL:HG13	2.46	0.50
1:B:281:ALA:O	1:B:284:THR:O	2.28	0.50
1:B:265:THR:CG2	1:B:267:PHE:CE1	2.93	0.50
1:B:317:VAL:O	1:B:320:ASN:O	2.30	0.50
1:B:126:LYS:HA	1:C:299:THR:HG21	1.94	0.50
1:C:246:PHE:CD1	1:C:246:PHE:O	2.65	0.50
1:B:320:ASN:OD1	1:B:320:ASN:O	2.30	0.50
1:C:198:ILE:O	1:C:202:LEU:HD13	2.11	0.50
1:B:218:SER:HA	1:B:267:PHE:O	2.11	0.50
1:C:173:PHE:O	1:C:174:VAL:C	2.50	0.50
1:C:143:ALA:CB	1:C:236:TYR:OH	2.60	0.50
1:A:94:THR:O	1:A:97:ASP:HB2	2.12	0.50
1:C:304:VAL:HG13	1:C:310:LEU:HB2	1.92	0.50
1:B:206:LEU:O	1:B:209:VAL:CG1	2.60	0.50
1:B:128:VAL:O	1:B:129:PRO:O	2.30	0.50
1:B:126:LYS:CG	1:C:299:THR:HG23	2.41	0.50
1:C:246:PHE:CE2	1:C:276:GLY:CA	2.93	0.50
1:A:312:GLU:OE1	4:A:332:CAC:O2	2.29	0.50
1:B:266:ILE:HD13	1:B:280:VAL:CG2	2.41	0.50
1:A:276:GLY:O	1:A:279:GLN:HB2	2.11	0.50
1:C:204:ALA:HA	1:C:207:GLU:CD	2.33	0.50
1:C:281:ALA:O	1:C:282:GLN:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:TYR:O	1:C:184:TYR:C	2.50	0.50
1:C:210:PRO:HG2	1:C:213:GLN:CD	2.33	0.50
1:C:278:LYS:O	1:C:281:ALA:O	2.30	0.50
1:A:126:LYS:O	1:A:128:VAL:HG23	2.12	0.49
1:B:112:MET:HG3	1:B:134:THR:HG21	1.94	0.49
1:A:244:GLN:O	1:A:245:GLN:O	2.30	0.49
1:B:222:ALA:HB1	1:B:294:VAL:HG11	1.95	0.49
1:B:98:ILE:HD12	1:B:124:ASN:ND2	2.27	0.49
1:B:255:ILE:CG2	1:B:280:VAL:HB	2.41	0.49
1:C:154:HIS:HA	1:C:156:TRP:CZ3	2.47	0.49
1:A:293:TYR:O	1:A:310:LEU:HD11	2.13	0.49
1:A:182:LYS:HE3	1:A:183:TYR:HE1	1.77	0.49
1:B:284:THR:C	1:B:286:ALA:H	2.16	0.49
1:A:137:ILE:CG1	1:A:164:VAL:HG21	2.33	0.49
1:C:194:GLN:HB3	1:C:308:LEU:HD21	1.94	0.49
1:A:260:THR:O	1:A:261:ASN:OD1	2.30	0.49
1:A:179:ASP:OD1	4:A:2327:CAC:C1	2.61	0.49
1:C:279:GLN:O	1:C:281:ALA:C	2.51	0.49
1:C:220:GLU:OE1	1:C:222:ALA:HB2	2.13	0.48
1:C:217:VAL:HG21	1:C:266:ILE:CB	2.43	0.48
1:B:108:LEU:HG	1:B:133:LEU:HD21	1.95	0.48
1:A:166:VAL:HA	1:A:169:ILE:HD12	1.95	0.48
1:B:125:VAL:O	1:B:126:LYS:O	2.30	0.48
1:A:304:VAL:HG13	1:A:310:LEU:CA	2.43	0.48
1:B:67:MET:HE1	1:B:165:TYR:CB	2.44	0.48
1:A:68:VAL:CG2	1:A:78:VAL:HG11	2.43	0.48
1:C:278:LYS:C	1:C:281:ALA:H	2.16	0.48
1:A:217:VAL:HA	1:A:235:ILE:O	2.13	0.48
1:C:132:VAL:HG22	1:C:134:THR:H	1.77	0.48
1:A:122:LEU:O	1:A:125:VAL:HG22	2.13	0.48
1:A:126:LYS:CG	1:A:127:ASP:N	2.73	0.48
1:C:65:ALA:CB	1:C:80:SER:HB2	2.40	0.48
1:B:88:ILE:HG12	1:B:295:ASP:HB3	1.94	0.48
1:B:134:THR:O	1:B:134:THR:HG23	2.12	0.48
1:A:58:LEU:CD2	1:A:81:ILE:HD11	2.41	0.48
1:C:147:TYR:N	1:C:147:TYR:HD1	2.10	0.48
1:B:317:VAL:HG22	1:B:318:ILE:N	2.29	0.48
1:A:134:THR:O	1:A:137:ILE:HG13	2.13	0.48
1:B:112:MET:CE	1:B:139:PRO:HB3	2.43	0.48
1:B:171:GLN:O	1:B:175:GLU:HG3	2.13	0.48
1:B:197:ALA:HA	1:B:200:ARG:HH21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:VAL:HG12	1:B:169:ILE:CD1	2.43	0.48
1:B:56:LYS:HG3	1:B:77:VAL:CG1	2.43	0.48
1:C:114:LEU:HB2	1:C:153:PRO:HB2	1.96	0.48
1:A:266:ILE:HD11	1:A:281:ALA:HB2	1.95	0.48
1:B:217:VAL:CG1	1:B:266:ILE:HG22	2.44	0.47
1:B:58:LEU:HD21	1:B:81:ILE:CD1	2.43	0.47
1:C:266:ILE:CD1	1:C:280:VAL:CG1	2.91	0.47
1:B:217:VAL:HG11	1:B:266:ILE:HG22	1.96	0.47
1:C:279:GLN:O	1:C:280:VAL:C	2.51	0.47
1:C:181:ALA:O	1:C:182:LYS:C	2.53	0.47
1:C:245:GLN:O	1:C:246:PHE:O	2.33	0.47
1:A:304:VAL:HG13	1:A:310:LEU:HB2	1.96	0.47
1:B:121:PHE:O	1:B:125:VAL:CG1	2.62	0.47
1:A:190:VAL:HG21	1:B:139:PRO:HG3	1.97	0.47
1:B:156:TRP:C	1:B:158:SER:H	2.17	0.47
1:A:51:THR:O	1:A:52:GLU:C	2.51	0.47
1:C:200:ARG:HB3	1:C:200:ARG:HH21	1.80	0.47
1:B:140:ILE:HG12	1:B:225:TYR:CE1	2.50	0.47
1:C:220:GLU:CB	1:C:241:ASN:OD1	2.56	0.47
1:C:223:PHE:N	1:C:223:PHE:CD1	2.83	0.47
1:A:125:VAL:O	1:A:125:VAL:CG2	2.62	0.47
1:C:276:GLY:O	1:C:279:GLN:HB2	2.15	0.47
1:B:304:VAL:HG12	1:B:304:VAL:O	2.15	0.47
1:B:88:ILE:HD12	1:B:114:LEU:HD21	1.95	0.46
1:C:266:ILE:CD1	1:C:277:GLN:HG3	2.45	0.46
1:C:142:ILE:CG2	1:C:143:ALA:H	2.15	0.46
1:A:269:GLU:HG2	1:A:294:VAL:CG2	2.45	0.46
1:A:198:ILE:O	1:A:202:LEU:HB2	2.15	0.46
1:B:219:CYS:O	1:B:238:TRP:CD2	2.68	0.46
1:B:198:ILE:HD11	1:B:311:LEU:CD1	2.42	0.46
1:C:182:LYS:O	1:C:183:TYR:C	2.53	0.46
1:B:264:PRO:HG2	1:B:322:LEU:HA	1.96	0.46
1:B:182:LYS:HG2	1:B:183:TYR:H	1.79	0.46
1:A:246:PHE:C	1:A:246:PHE:CD1	2.88	0.46
1:A:147:TYR:HB3	1:A:150:LYS:HB2	1.98	0.46
1:C:146:PRO:HB2	1:C:147:TYR:CD1	2.50	0.46
1:B:240:ILE:HG23	1:B:241:ASN:N	2.28	0.46
1:B:98:ILE:HD12	1:B:124:ASN:HD21	1.79	0.46
1:C:201:GLN:NE2	1:C:312:GLU:CG	2.79	0.46
1:C:223:PHE:O	1:C:225:TYR:N	2.49	0.46
1:C:307:PHE:CE2	1:C:311:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:CD1	1:B:323:LEU:N	2.78	0.46
1:A:87:GLU:OE1	1:A:89:HIS:HB2	2.16	0.46
1:B:238:TRP:CZ2	1:B:272:VAL:HG21	2.51	0.46
1:C:98:ILE:HG12	1:C:121:PHE:CE1	2.51	0.46
1:A:140:ILE:HD11	1:A:228:ARG:NH2	2.31	0.45
1:A:242:ALA:O	1:A:243:GLU:HB2	2.15	0.45
1:B:235:ILE:HG22	1:B:254:VAL:HG13	1.98	0.45
1:B:257:GLU:O	1:B:258:VAL:C	2.55	0.45
1:C:173:PHE:C	1:C:175:GLU:N	2.69	0.45
1:C:158:SER:O	1:C:161:ASN:N	2.49	0.45
1:B:263:VAL:HA	1:B:264:PRO:HD2	1.80	0.45
1:C:204:ALA:HA	1:C:207:GLU:OE2	2.16	0.45
1:A:83:ARG:HH11	1:A:100:LYS:NZ	2.14	0.45
1:A:132:VAL:C	1:A:134:THR:H	2.20	0.45
1:B:112:MET:HE3	1:B:139:PRO:HB3	1.98	0.45
1:A:190:VAL:HG22	1:B:112:MET:HG2	1.97	0.45
1:A:64:LEU:HD13	1:A:133:LEU:HD12	1.97	0.45
1:B:244:GLN:C	1:B:246:PHE:H	2.18	0.45
1:B:201:GLN:OE1	1:B:316:ARG:NH1	2.45	0.45
1:C:161:ASN:O	1:C:164:VAL:HG22	2.17	0.45
1:B:158:SER:O	1:B:161:ASN:HB2	2.17	0.45
1:A:68:VAL:HG23	1:A:78:VAL:HG11	1.99	0.45
1:C:77:VAL:HG22	1:C:77:VAL:O	2.16	0.45
1:C:125:VAL:HB	1:C:128:VAL:HG23	1.98	0.45
1:B:56:LYS:HE2	5:B:14:HOH:O	2.16	0.45
1:B:284:THR:O	1:B:286:ALA:N	2.44	0.45
1:C:114:LEU:HD11	1:C:156:TRP:HH2	1.81	0.45
1:B:137:ILE:CD1	1:B:164:VAL:CG2	2.80	0.45
1:B:255:ILE:HG21	1:B:280:VAL:HA	1.91	0.45
1:C:147:TYR:HB3	1:C:150:LYS:CG	2.41	0.45
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.61	0.44
1:A:312:GLU:OE2	4:A:332:CAC:AS	2.94	0.44
1:C:293:TYR:CD1	1:C:304:VAL:HG21	2.52	0.44
1:B:214:ARG:N	1:B:215:PHE:CD1	2.85	0.44
1:A:210:PRO:HG2	1:A:213:GLN:CD	2.37	0.44
1:C:237:MET:SD	1:C:246:PHE:CD2	3.11	0.44
1:A:277:GLN:HA	1:A:277:GLN:NE2	2.28	0.44
1:A:195:LEU:HD13	1:A:308:LEU:HD11	1.99	0.44
1:C:171:GLN:O	1:C:174:VAL:HG22	2.17	0.44
1:C:84:ILE:O	1:C:85:GLY:C	2.56	0.44
1:B:233:GLU:HG3	1:B:234:GLU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASP:HB3	5:B:18:HOH:O	2.16	0.44
1:C:217:VAL:HG21	1:C:266:ILE:HB	1.99	0.44
1:A:158:SER:O	1:A:161:ASN:N	2.50	0.44
1:A:87:GLU:HG3	1:A:87:GLU:O	2.16	0.44
1:A:132:VAL:HG23	1:A:134:THR:H	1.83	0.44
1:C:217:VAL:CG2	1:C:266:ILE:HB	2.48	0.43
1:A:154:HIS:HB3	1:A:222:ALA:O	2.18	0.43
1:B:296:SER:OG	1:B:297:LEU:N	2.51	0.43
1:C:298:SER:O	1:C:305:PRO:HA	2.18	0.43
1:B:273:SER:OG	1:B:275:LYS:HG3	2.18	0.43
1:B:101:ALA:HB2	1:B:121:PHE:CZ	2.53	0.43
1:C:259:LYS:CG	1:C:284:THR:OG1	2.39	0.43
1:C:220:GLU:CD	1:C:222:ALA:HB2	2.39	0.43
1:C:278:LYS:HA	1:C:281:ALA:CB	2.45	0.43
1:A:220:GLU:O	1:A:222:ALA:N	2.46	0.43
1:B:71:VAL:HG11	1:B:169:ILE:HG22	2.00	0.43
1:C:52:GLU:HG3	1:C:53:GLU:N	2.33	0.43
1:C:244:GLN:HB3	1:C:245:GLN:H	1.58	0.43
1:A:137:ILE:HD11	1:A:164:VAL:HG23	2.00	0.43
1:A:102:GLN:HG2	1:A:102:GLN:H	1.58	0.43
1:C:98:ILE:HG12	1:C:121:PHE:CD1	2.53	0.43
1:C:57:VAL:HG12	1:C:58:LEU:N	2.34	0.43
1:A:224:SER:OG	1:A:234:GLU:OE2	2.32	0.43
1:B:267:PHE:HB3	1:B:292:LEU:HG	2.01	0.43
1:A:139:PRO:HA	1:A:225:TYR:OH	2.17	0.43
1:B:284:THR:HG23	1:B:286:ALA:CB	2.48	0.43
1:C:258:VAL:HG23	1:C:263:VAL:HB	2.01	0.43
1:B:200:ARG:O	1:B:201:GLN:C	2.57	0.43
1:B:89:HIS:NE2	1:B:220:GLU:OE2	2.52	0.43
1:A:88:ILE:HD12	1:A:114:LEU:HD21	2.00	0.43
1:B:282:GLN:HE21	1:B:282:GLN:HB2	1.63	0.43
1:B:280:VAL:HG22	1:B:281:ALA:N	2.34	0.43
1:C:122:LEU:HD12	1:C:125:VAL:HG21	1.99	0.43
1:C:279:GLN:C	1:C:281:ALA:H	2.18	0.43
1:C:213:GLN:O	1:C:322:LEU:HD13	2.18	0.43
1:A:307:PHE:CZ	1:A:311:LEU:HD11	2.54	0.43
1:B:239:PRO:HG2	1:B:240:ILE:H	1.84	0.42
1:B:58:LEU:HA	1:B:79:GLU:O	2.19	0.42
1:C:97:ASP:N	1:C:97:ASP:OD2	2.52	0.42
1:B:237:MET:HE1	1:B:238:TRP:HZ3	1.84	0.42
1:B:122:LEU:O	1:B:125:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:O	1:A:280:VAL:CG2	2.67	0.42
1:B:211:ALA:HA	1:B:214:ARG:NE	2.33	0.42
1:B:267:PHE:CE2	1:B:317:VAL:CG2	3.02	0.42
1:B:158:SER:O	1:B:161:ASN:N	2.48	0.42
1:C:223:PHE:O	1:C:224:SER:C	2.57	0.42
1:C:304:VAL:O	1:C:304:VAL:HG12	2.19	0.42
1:B:98:ILE:H	1:B:98:ILE:HG12	1.59	0.42
1:C:266:ILE:CD1	1:C:280:VAL:HB	2.50	0.42
1:A:140:ILE:HG12	1:A:225:TYR:CE1	2.55	0.42
1:A:259:LYS:O	1:A:261:ASN:N	2.53	0.42
1:A:112:MET:CG	1:A:134:THR:HG21	2.36	0.42
1:A:112:MET:HE2	1:A:139:PRO:HB3	1.90	0.42
1:C:201:GLN:HE21	1:C:312:GLU:HG3	1.82	0.42
1:C:105:ASP:O	1:C:106:LEU:HB2	2.20	0.42
1:C:266:ILE:HD12	1:C:280:VAL:HB	2.01	0.42
1:A:258:VAL:HG12	1:A:259:LYS:H	1.77	0.42
1:A:110:ASN:C	1:A:110:ASN:HD22	2.23	0.42
1:B:279:GLN:HA	1:B:282:GLN:HG2	2.02	0.42
1:B:245:GLN:HA	1:B:245:GLN:OE1	2.20	0.42
1:C:295:ASP:O	1:C:296:SER:CB	2.68	0.42
1:A:101:ALA:HB2	1:A:121:PHE:CZ	2.55	0.42
1:B:218:SER:O	1:B:236:TYR:HA	2.20	0.42
1:C:278:LYS:O	1:C:279:GLN:C	2.57	0.42
1:C:121:PHE:C	1:C:123:GLY:N	2.71	0.42
1:C:177:ASP:CG	1:C:180:ASN:HD22	2.22	0.42
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.79	0.42
1:A:170:ARG:HG3	1:A:188:ALA:HB2	2.01	0.42
1:B:255:ILE:HG13	1:B:255:ILE:H	1.70	0.42
1:A:154:HIS:CD2	1:A:222:ALA:HB1	2.54	0.42
1:C:248:PRO:O	1:C:252:GLN:HB2	2.20	0.41
1:A:137:ILE:HG12	1:A:164:VAL:CG2	2.33	0.41
1:C:223:PHE:CE2	1:C:294:VAL:CG1	3.03	0.41
1:B:148:THR:HG23	1:B:149:ASP:N	2.34	0.41
1:A:77:VAL:O	1:A:77:VAL:HG22	2.20	0.41
1:C:64:LEU:HD13	1:C:133:LEU:HD12	2.02	0.41
1:A:147:TYR:HA	1:A:150:LYS:HG2	2.02	0.41
1:A:98:ILE:HG21	1:A:124:ASN:HD21	1.78	0.41
1:C:111:GLY:O	1:C:112:MET:HB2	2.21	0.41
1:B:58:LEU:CD2	1:B:81:ILE:HD11	2.48	0.41
1:C:205:ASP:O	1:C:208:GLN:HG3	2.21	0.41
1:C:190:VAL:O	1:C:193:GLU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:C	1:B:256:GLU:N	2.73	0.41
1:B:310:LEU:HD23	1:B:310:LEU:C	2.41	0.41
1:B:244:GLN:C	1:B:246:PHE:N	2.74	0.41
1:B:323:LEU:HD12	1:B:323:LEU:N	2.35	0.41
1:C:277:GLN:O	1:C:280:VAL:HB	2.21	0.41
1:A:127:ASP:O	1:A:128:VAL:HG23	2.20	0.41
1:C:250:GLN:C	1:C:252:GLN:N	2.73	0.41
1:A:191:TYR:HE1	1:A:308:LEU:HD22	1.86	0.41
1:A:304:VAL:HG13	1:A:310:LEU:CB	2.51	0.41
1:B:157:MET:HG2	1:B:294:VAL:HG12	2.03	0.41
1:A:226:LEU:HA	1:A:226:LEU:HD12	1.69	0.41
1:C:316:ARG:H	1:C:316:ARG:HG3	1.52	0.41
1:C:220:GLU:HB2	1:C:238:TRP:HE1	1.85	0.41
1:A:253:THR:O	1:A:256:GLU:HG2	2.21	0.41
1:B:258:VAL:O	1:B:262:ASN:CA	2.65	0.40
1:B:124:ASN:CB	1:C:84:ILE:HG22	2.51	0.40
1:B:67:MET:HB3	1:B:67:MET:HE3	1.88	0.40
1:A:118:PHE:O	1:A:119:GLU:C	2.59	0.40
1:A:320:ASN:C	1:A:320:ASN:ND2	2.74	0.40
1:C:128:VAL:HA	1:C:129:PRO:HD2	1.76	0.40
1:C:58:LEU:HA	1:C:58:LEU:HD12	1.84	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	272/307 (89%)	233 (86%)	33 (12%)	6 (2%)	8	22
1	B	263/307 (86%)	222 (84%)	31 (12%)	10 (4%)	4	9
1	C	270/307 (88%)	215 (80%)	32 (12%)	23 (8%)	1	1
All	All	805/921 (87%)	670 (83%)	96 (12%)	39 (5%)	3	5

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	85	GLY
1	A	154	HIS
1	A	243	GLU
1	A	245	GLN
1	B	126	LYS
1	B	129	PRO
1	B	200	ARG
1	B	246	PHE
1	C	84	ILE
1	C	126	LYS
1	C	127	ASP
1	C	146	PRO
1	C	246	PHE
1	C	282	GLN
1	B	83	ARG
1	B	127	ASP
1	B	242	ALA
1	B	290	GLY
1	C	85	GLY
1	C	174	VAL
1	C	182	LYS
1	C	183	TYR
1	C	184	TYR
1	C	221	GLY
1	C	283	ALA
1	C	284	THR
1	B	201	GLN
1	C	135	GLU
1	C	242	ALA
1	C	244	GLN
1	C	296	SER
1	A	52	GLU
1	C	224	SER
1	C	280	VAL
1	B	157	MET
1	C	106	LEU
1	C	285	GLY
1	C	142	ILE

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	234/259 (90%)	195 (83%)	39 (17%)	3	7
1	B	229/259 (88%)	181 (79%)	48 (21%)	1	3
1	C	233/259 (90%)	193 (83%)	40 (17%)	2	6
All	All	696/777 (90%)	569 (82%)	127 (18%)	2	5

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

Mol	Chain	Res	Type
1	A	56	LYS
1	A	77	VAL
1	A	98	ILE
1	A	102	GLN
1	A	103	ASP
1	A	108	LEU
1	A	110	ASN
1	A	115	GLU
1	A	134	THR
1	A	138	GLU
1	A	148	THR
1	A	149	ASP
1	A	150	LYS
1	A	160	ARG
1	A	195	LEU
1	A	199	ASP
1	A	201	GLN
1	A	202	LEU
1	A	205	ASP
1	A	209	VAL
1	A	216	LEU
1	A	217	VAL
1	A	244	GLN
1	A	247	THR
1	A	258	VAL
1	A	260	THR

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Mol	Chain	Res	Type
1	A	268	CYS
1	A	277	GLN
1	A	280	VAL
1	A	282	GLN
1	A	284	THR
1	A	287	ARG
1	A	294	VAL
1	A	296	SER
1	A	298	SER
1	A	308	LEU
1	A	320	ASN
1	A	322	LEU
1	A	323	LEU
1	B	56	LYS
1	B	68	VAL
1	B	83	ARG
1	B	84	ILE
1	B	87	GLU
1	B	96	SER
1	B	98	ILE
1	B	108	LEU
1	B	115	GLU
1	B	120	GLN
1	B	124	ASN
1	B	125	VAL
1	B	127	ASP
1	B	130	SER
1	B	131	VAL
1	B	134	THR
1	B	135	GLU
1	B	140	ILE
1	B	157	MET
1	B	158	SER
1	B	166	VAL
1	B	182	LYS
1	B	185	ASN
1	B	195	LEU
1	B	198	ILE
1	B	199	ASP
1	B	200	ARG
1	B	205	ASP
1	B	214	ARG

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Mol	Chain	Res	Type
1	B	215	PHE
1	B	217	VAL
1	B	228	ARG
1	B	240	ILE
1	B	243	GLU
1	B	251	VAL
1	B	256	GLU
1	B	259	LYS
1	B	265	THR
1	B	277	GLN
1	B	282	GLN
1	B	287	ARG
1	B	294	VAL
1	B	299	THR
1	B	300	GLU
1	B	308	LEU
1	B	317	VAL
1	B	318	ILE
1	B	319	THR
1	C	68	VAL
1	C	77	VAL
1	C	84	ILE
1	C	87	GLU
1	C	94	THR
1	C	96	SER
1	C	97	ASP
1	C	108	LEU
1	C	110	ASN
1	C	124	ASN
1	C	127	ASP
1	C	128	VAL
1	C	131	VAL
1	C	134	THR
1	C	138	GLU
1	C	144	ASP
1	C	147	TYR
1	C	150	LYS
1	C	166	VAL
1	C	175	GLU
1	C	182	LYS
1	C	205	ASP
1	C	207	GLU

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Mol	Chain	Res	Type
1	C	208	GLN
1	C	209	VAL
1	C	217	VAL
1	C	218	SER
1	C	229	ASP
1	C	240	ILE
1	C	243	GLU
1	C	245	GLN
1	C	246	PHE
1	C	251	VAL
1	C	273	SER
1	C	277	GLN
1	C	279	GLN
1	C	287	ARG
1	C	299	THR
1	C	316	ARG
1	C	317	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	124	ASN
1	A	161	ASN
1	A	201	GLN
1	A	277	GLN
1	B	120	GLN
1	B	124	ASN
1	B	161	ASN
1	B	185	ASN
1	B	261	ASN
1	B	277	GLN
1	B	282	GLN
1	C	89	HIS
1	C	161	ASN
1	C	180	ASN
1	C	185	ASN
1	C	201	GLN
1	C	213	GLN
1	C	277	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	CAC	A	2327	-	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	A	332	-	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	C	2327	-	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	C	332	-	0,4,4	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAC	A	2327	-	-	0/0/0/0	0/0/0/0
4	CAC	A	332	-	-	0/0/0/0	0/0/0/0
4	CAC	C	2327	-	-	0/0/0/0	0/0/0/0
4	CAC	C	332	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2327	CAC	1	0
4	A	332	CAC	3	0

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	274/307 (89%)	0.13	5 (1%) 71	72	59, 77, 102, 116	0
1	B	267/307 (86%)	0.27	11 (4%) 41	41	54, 83, 120, 131	0
1	C	272/307 (88%)	0.51	22 (8%) 15	12	24, 95, 136, 162	0
All	All	813/921 (88%)	0.31	38 (4%) 35	34	24, 83, 129, 162	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	TYR	4.5
1	B	259	LYS	4.5
1	B	217	VAL	3.6
1	C	275	LYS	3.6
1	C	254	VAL	3.5
1	C	200	ARG	3.4
1	A	126	LYS	3.3
1	C	319	THR	3.2
1	C	53	GLU	3.1
1	C	265	THR	3.0
1	C	60	THR	2.9
1	B	128	VAL	2.9
1	B	142	ILE	2.8
1	B	126	LYS	2.7
1	C	268	CYS	2.7
1	C	311	LEU	2.7
1	C	88	ILE	2.7
1	A	242	ALA	2.7
1	B	234	GLU	2.6
1	C	143	ALA	2.6
1	C	323	LEU	2.5
1	C	242	ALA	2.5
1	C	206	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	247	THR	2.4
1	B	282	GLN	2.4
1	C	266	ILE	2.4
1	C	236	TYR	2.3
1	C	281	ALA	2.3
1	B	216	LEU	2.3
1	C	52	GLU	2.2
1	B	312	GLU	2.2
1	A	127	ASP	2.2
1	B	125	VAL	2.1
1	C	233	GLU	2.1
1	C	302	GLY	2.1
1	A	140	ILE	2.1
1	A	244	GLN	2.0
1	C	310	LEU	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	ZN	C	4	1/1	0.94	0.35	2.75	111,111,111,111	0
3	ZN	C	331	1/1	0.47	0.34	1.55	133,133,133,133	0
2	MN	B	1	1/1	1.00	0.18	0.00	64,64,64,64	0
2	MN	A	1	1/1	0.99	0.19	-0.20	56,56,56,56	0
3	ZN	A	2	1/1	0.93	0.15	-0.29	88,88,88,88	1
4	CAC	A	332	5/5	0.91	0.17	-0.33	68,83,91,114	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	MN	C	1	1/1	0.99	0.08	-1.69	85,85,85,85	0
4	CAC	A	2327	5/5	0.66	0.17	-	133,134,149,199	0
3	ZN	A	331	1/1	0.93	0.18	-	113,113,113,113	0
4	CAC	C	332	5/5	0.85	0.18	-	127,139,141,166	1
3	ZN	A	5	1/1	0.93	0.04	-	142,142,142,142	0
3	ZN	A	3	1/1	0.90	0.09	-	110,110,110,110	1
4	CAC	C	2327	5/5	0.86	0.13	-	98,102,111,143	1

6.5 Other polymers (i)

There are no such residues in this entry.