



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:50 AM UTC

PDB ID : 3UJP / pdb_00003ujp
Title : Structure of MntC protein at 2.7Å
Authors : Kanteev, M.; Adir, N.
Deposited on : 2011-11-08
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

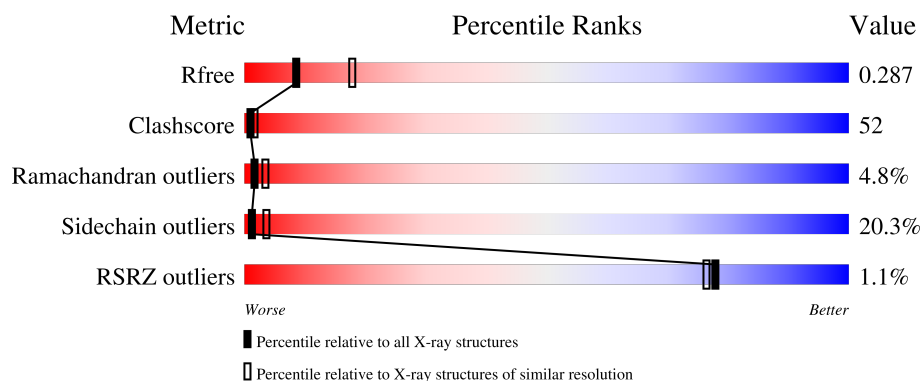
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	307	37% 41% 9% 11%
1	B	307	32% 38% 15% 13%
1	C	307	30% 40% 16% 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
4	CAC	A	2327	-	X	-	-
4	CAC	A	332	-	X	-	-
4	CAC	C	2327	-	X	-	-
4	CAC	C	332	-	X	-	-

2 Entry composition

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	C	N	O	S	0	0	0
			2149	1365	352	425	7			
1	B	267	Total	C	N	O	S	0	0	0
			2097	1333	345	412	7			
1	C	272	Total	C	N	O	S	0	0	0
			2137	1358	350	422	7			

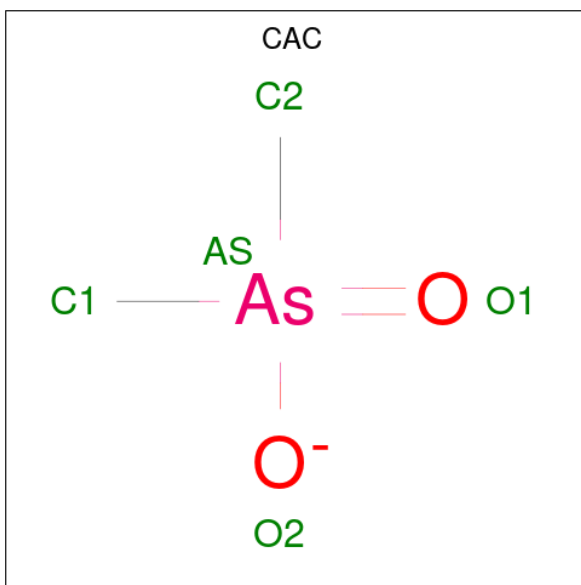
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		

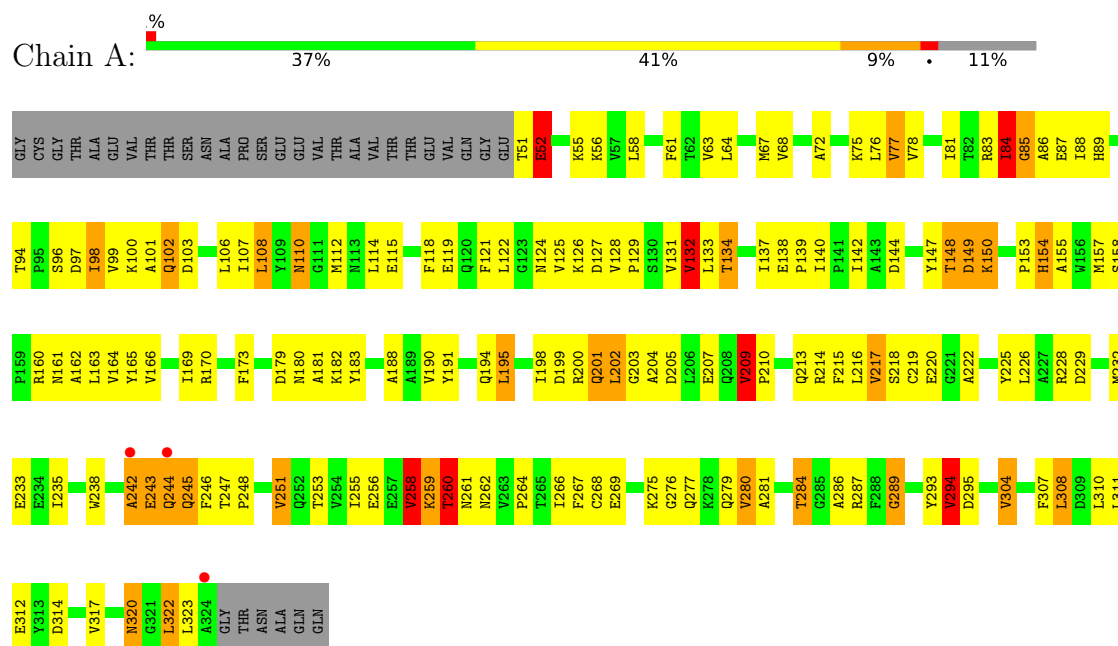
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	5	Total	O	0	0
			5	5		
5	C	1	Total	O	0	0
			1	1		

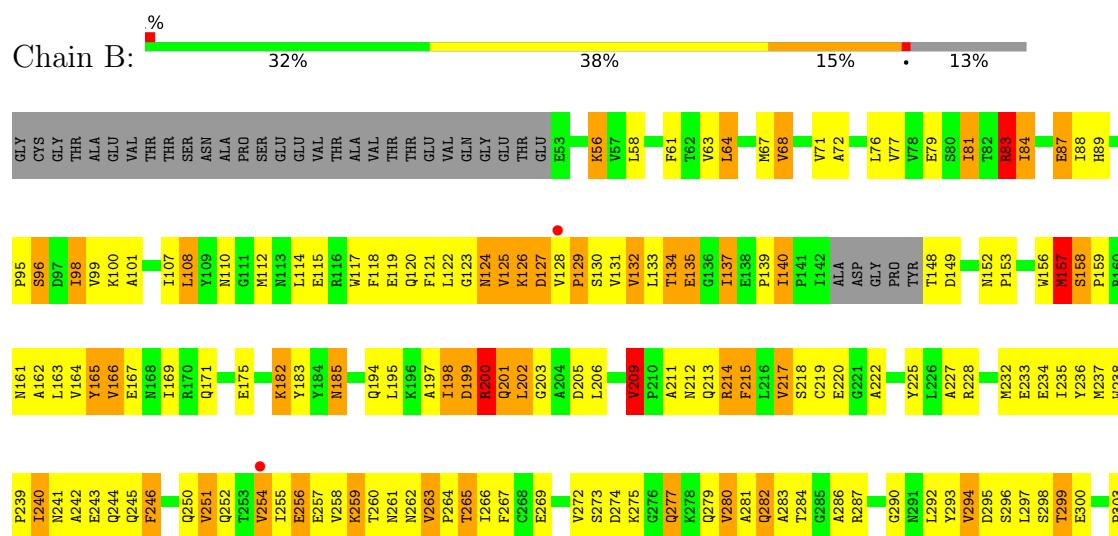
3 Residue-property plots

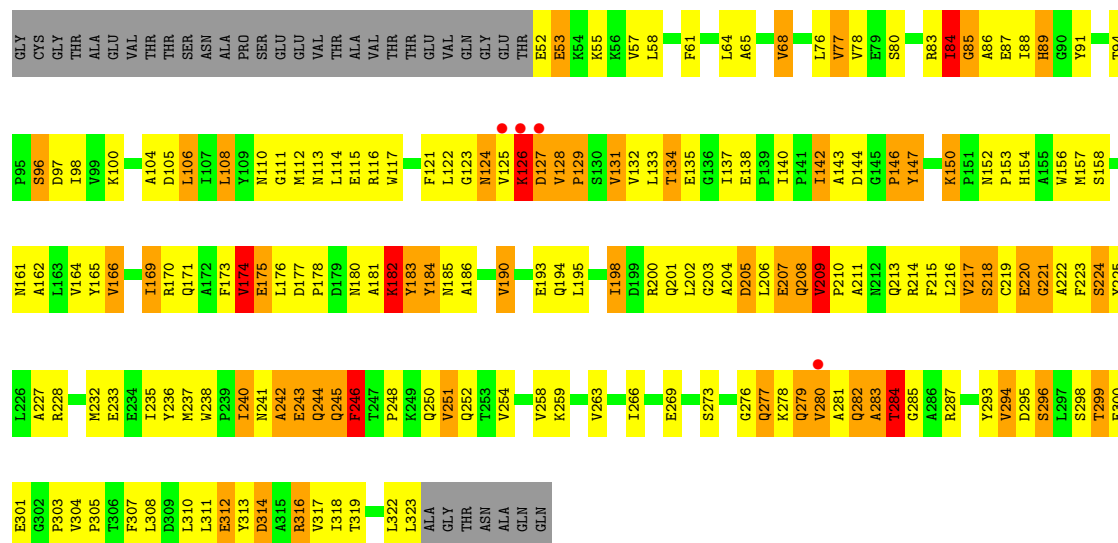
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Mn transporter subunit



• Molecule 1: Mn transporter subunit





4 Data and refinement statistics

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 36.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.0 (36.80-2.70) 91.9 (36.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.231 , 0.284 0.239 , 0.287	Depositor DCC
R_{free} test set	1090 reflections (5.05%)	wwPDB-VP
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 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	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.*

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

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

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	0.78	1/2194 (0.0%)	1.13	11/2991 (0.4%)
1	B	0.88	1/2139 (0.0%)	1.09	7/2913 (0.2%)
1	C	0.72	1/2182 (0.0%)	1.02	6/2974 (0.2%)
All	All	0.80	3/6515 (0.0%)	1.08	24/8878 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	GLY	C-N	-9.34	1.22	1.33
1	C	129	PRO	C-N	-6.88	1.24	1.33
1	A	132	VAL	CA-CB	6.17	1.61	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	HIS	N-CA-C	-9.94	100.45	111.28
1	A	260	THR	N-CA-C	-8.93	101.49	112.38
1	C	314	ASP	N-CA-C	-8.14	102.41	111.28
1	A	294	VAL	CB-CA-C	-8.06	103.88	111.05
1	A	289	GLY	N-CA-C	-7.91	103.63	112.33
1	A	259	LYS	N-CA-C	-7.74	102.85	111.28
1	B	263	VAL	N-CA-C	7.69	115.16	107.55
1	A	209	VAL	CA-C-N	7.37	127.13	119.76
1	A	209	VAL	C-N-CA	7.37	127.13	119.76
1	B	209	VAL	CA-C-N	6.72	126.70	119.78
1	B	209	VAL	C-N-CA	6.72	126.70	119.78
1	C	312	GLU	N-CA-C	-6.62	103.99	111.07
1	A	258	VAL	CB-CA-C	-6.53	103.47	112.02
1	A	144	ASP	N-CA-C	6.14	116.18	108.45
1	C	152	ASN	CA-C-N	5.90	125.52	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ASN	C-N-CA	5.90	125.52	119.56
1	B	63	VAL	N-CA-C	-5.81	104.67	111.00
1	A	75	LYS	N-CA-C	5.70	118.43	111.82
1	C	209	VAL	N-CA-C	-5.66	102.74	108.96
1	B	165	TYR	N-CA-C	-5.63	105.06	111.14
1	A	242	ALA	N-CA-C	5.58	122.42	114.16
1	A	294	VAL	N-CA-C	5.36	115.85	111.62
1	B	81	ILE	N-CA-C	5.24	115.86	110.36
1	B	263	VAL	CB-CA-C	-5.08	105.04	111.04

There are no chirality outliers.

There are no planarity outliers.

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	2149	0	2097	175	0
1	B	2097	0	2055	255	0
1	C	2137	0	2087	242	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
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	657	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 52.

All (657) 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:A:148:THR:HG22	1:A:149:ASP:N	1.72	1.01
1:C:170:ARG:O	1:C:174:VAL:HG13	1.60	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:HE21	1:C:277:GLN:HA	1.25	0.98
1:C:278:LYS:O	1:C:281:ALA:HB3	1.64	0.98
1:C:284:THR:O	1:C:284:THR:HG22	1.63	0.97
1:C:281:ALA:O	1:C:282:GLN:HG3	1.63	0.97
1:B:263:VAL:HG23	1:B:263:VAL:O	1.63	0.97
1:A:258:VAL:HG12	1:A:259:LYS:N	1.78	0.96
1:B:125:VAL:HG22	1:B:125:VAL:O	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:B:238:TRP:CG	1:B:244:GLN:HE21	1.83	0.94
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:A:112:MET:HG3	1:A:134:THR:HG21	1.48	0.92
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:C:219:CYS:HB3	1:C:238:TRP:CH2	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:242:ALA:C	1:A:243:GLU:HG2	1.97	0.89
1:B:238:TRP:CG	1:B:244:GLN:NE2	2.41	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: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:B:185:ASN:N	1:B:185:ASN:HD22	1.72	0.84
1:C:220:GLU:HB2	1:C:241:ASN:OD1	1.77	0.84
1:B:137:ILE:HD11	1:B:164:VAL:HG23	1.61	0.83
1:B:238:TRP:NE1	1:B:244:GLN:NE2	2.26	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
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:125:VAL:O	1:C:126:LYS:C	2.23	0.82
1:C:175:GLU:O	1:C:178:PRO:HD3	1.80	0.82
1:C:259:LYS:HG2	1:C:284:THR:HG1	1.45	0.81
1:A:280:VAL:O	1:A:284:THR:HB	1.79	0.81
1:B:258:VAL:HG22	1:B:263:VAL:HG21	1.61	0.81
1:B:238:TRP:CD1	1:B:244:GLN:HE21	1.97	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:B:240:ILE:CG2	1:B:241:ASN:O	2.30	0.80
1:C:283:ALA:O	1:C:284:THR:HB	1.82	0.80
1:C:284:THR:O	1:C:284:THR:CG2	2.30	0.80
1:C:96:SER:O	1:C:100:LYS:HG2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:TYR:HB3	1:C:150:LYS:HG3	1.63	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:O	1:C:217:VAL:CG2	2.30	0.79
1:A:96:SER:O	1:A:99:VAL:HG12	1.82	0.78
1:B:110:ASN:O	1:B:134:THR:HB	1.83	0.78
1:C:246:PHE:CE2	1:C:276:GLY:HA3	2.19	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:B:238:TRP:NE1	1:B:244:GLN:HE22	1.81	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:HD12	1:B:137:ILE:N	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:N	1:B:185:ASN:ND2	2.31	0.76
1:A:154:HIS:CE1	1:A:220:GLU:OE2	2.39	0.75
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:107:ILE:CD1	1:B:128:VAL:HG11	2.17	0.74
1:B:258:VAL:HG11	1:B:286:ALA:HB2	1.69	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:C:127:ASP:C	1:C:128:VAL:HG22	2.14	0.73
1:B:263:VAL:CG2	1:B:263:VAL:O	2.35	0.73
1:B:215:PHE:CD1	1:B:215:PHE:N	2.55	0.72
1:B:280:VAL:O	1:B:284:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:HE1	1:A:139:PRO:HB3	1.71	0.72
1:C:122:LEU:O	1:C:125:VAL:HG22	1.89	0.71
1:C:278:LYS:O	1:C:281:ALA:C	2.34	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:A:88:ILE:HG12	1:A:295:ASP:HB3	1.73	0.70
1:C:108:LEU:HD12	1:C:131:VAL:HG13	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: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:67:MET:HE1	1:B:165:TYR:HB3	1.74	0.69
1:B:258:VAL:O	1:B:262:ASN:HA	1.93	0.69
1:C:244:GLN:C	1:C:245:GLN:HG2	2.18	0.69
1:C:279:GLN:C	1:C:281:ALA:N	2.48	0.69
1:A:67:MET:HE1	1:A:165:TYR:HB3	1.75	0.69
1:C:147:TYR:CB	1:C:150:LYS:HG3	2.23	0.69
1:A:218:SER:HA	1:A:267:PHE:O	1.93	0.69
1:C:183:TYR:O	1:C:186:ALA:N	2.25	0.69
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:B:137:ILE:CD1	1:B:164:VAL:HG21	2.24	0.68
1:C:55:LYS:HB2	1:C:76:LEU:HD22	1.76	0.68
1:C:217:VAL:HA	1:C:235:ILE:O	1.93	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:HA	1:B:83:ARG:HE	1.59	0.67
1:A:161:ASN:O	1:A:164:VAL:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:201:GLN:O	1:A:201:GLN:HG3	1.94	0.67
1:B:132:VAL:HG23	1:B:134:THR:H	1.58	0.67
1:B:126:LYS:O	1:B:127:ASP:C	2.36	0.67
1:B:157:MET:HE2	1:B:294:VAL:HG13	1.76	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:185:ASN:ND2	1:B:185:ASN:H	1.92	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:64:LEU:HD13	1:B:133:LEU:HD12	1.78	0.66
1:C:278:LYS:C	1:C:281:ALA:HB3	2.20	0.66
1:C:224:SER:O	1:C:227:ALA:HB3	1.96	0.66
1:B:137:ILE:HD11	1:B:164:VAL:HG21	1.74	0.65
1:C:218:SER:OG	1:C:219:CYS:N	2.28	0.65
1:B:198:ILE:HD12	1:B:198:ILE:O	1.96	0.65
1:B:128:VAL:O	1:B:129:PRO:C	2.39	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:A:108:LEU:HG	1:A:133:LEU:HD21	1.77	0.65
1:C:154:HIS:CG	1:C:222:ALA:CB	2.74	0.65
1:A:153:PRO:O	1:A:155:ALA:N	2.30	0.65
1:C:278:LYS:O	1:C:281:ALA:N	2.30	0.65
1:C:180:ASN:HB2	1:C:184:TYR:CE2	2.31	0.65
1:C:248:PRO:HA	1:C:251:VAL:CG1	2.22	0.65
1:B:251:VAL:O	1:B:255:ILE:CG1	2.45	0.64
1:B:198:ILE:HD12	1:B:198:ILE:C	2.23	0.64
1:C:220:GLU:O	1:C:220:GLU:CG	2.36	0.64
1:A:277:GLN:HE21	1:A:277:GLN:HA	1.62	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:98:ILE:HG21	1:A:124:ASN:ND2	2.13	0.64
1:A:126:LYS:O	1:A:127:ASP:C	2.39	0.64
1:B:265:THR:CB	1:B:321:GLY:O	2.32	0.64
1:B:61:PHE:CE2	1:B:64:LEU:HG	2.32	0.64
1:B:182:LYS:HG2	1:B:183:TYR:N	2.12	0.63
1:C:142:ILE:HG13	1:C:150:LYS:O	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:OE1	1:B:261:ASN:ND2	2.32	0.63
1:B:237:MET:HE2	1:B:238:TRP:HZ3	1.63	0.63
1:A:58:LEU:HD23	1:A:81:ILE:HD11	1.79	0.63
1:A:198:ILE:C	1:A:198:ILE:HD12	2.24	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:58:LEU:HD21	1:B:81:ILE:HD11	1.81	0.63
1:B:72:ALA:HB1	1:B:76:LEU:HB2	1.80	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:A:312:GLU:OE2	4:A:332:CAC:C1	2.47	0.62
1:B:107:ILE:HD12	1:B:128:VAL:HG12	1.81	0.62
1:B:255:ILE:HG22	1:B:280:VAL:CA	2.27	0.62
1:C:124:ASN:N	1:C:124:ASN:OD1	2.31	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:B:237:MET:HE2	1:B:238:TRP:CZ3	2.34	0.62
1:C:125:VAL:HB	1:C:128:VAL:HG21	1.82	0.62
1:C:217:VAL:O	1:C:217:VAL:HG23	1.99	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:C:142:ILE:HG22	1:C:143:ALA:N	2.08	0.62
1:B:122:LEU:HA	1:B:125:VAL:HG13	1.81	0.61
1:B:258:VAL:CG2	1:B:263:VAL:HG22	2.28	0.61
1:B:64:LEU:O	1:B:68:VAL:HG13	2.01	0.61
1:C:220:GLU:O	1:C:221:GLY:C	2.42	0.61
1:A:218:SER:HB2	1:A:269:GLU:OE2	2.01	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:C:217:VAL:O	1:C:217:VAL:HG22	2.00	0.60
1:B:256:GLU:HG3	1:B:257:GLU:N	2.15	0.60
1:B:304:VAL:HG13	1:B:310:LEU:HA	1.82	0.60
1:C:126:LYS:O	1:C:128:VAL:N	2.30	0.60
1:A:154:HIS:CE1	1:A:220:GLU:CD	2.79	0.60
1:A:261:ASN:O	1:A:262:ASN:C	2.42	0.60
1:B:265:THR:HG22	1:B:267:PHE:CE1	2.37	0.59
1:B:260:THR:HG23	1:B:261:ASN:ND2	2.17	0.59
1:C:200:ARG:NH2	1:C:200:ARG:HB3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:243:GLU:HG2	1:C:244:GLN:N	2.16	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: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:O	1:B:87:GLU:HG3	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: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:A:217:VAL:HG13	1:A:266:ILE:HA	1.86	0.58
1:C:84:ILE:O	1:C:86:ALA:N	2.36	0.58
1:B:220:GLU:CD	1:B:241:ASN:OD1	2.47	0.58
1:A:160:ARG:HG3	1:A:229:ASP:OD2	2.04	0.57
1:C:68:VAL:HG12	1:C:169:ILE:HD13	1.86	0.57
1:C:116:ARG:NH2	1:C:242:ALA:HA	2.19	0.57
1:C:201:GLN:HE22	1:C:312:GLU:CD	2.09	0.57
1:C:217:VAL:HG21	1:C:266:ILE:CG2	2.33	0.57
1:B:121:PHE:O	1:B:125:VAL:HG12	2.04	0.57
1:A:98:ILE:CG2	1:A:124:ASN:ND2	2.67	0.57
1:B:258:VAL:CB	1:B:263:VAL:HG22	2.35	0.57
1:B:95:PRO:HA	1:B:98:ILE:HG13	1.87	0.57
1:B:212:ASN:O	1:B:215:PHE:HZ	1.88	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:B:112:MET:HE3	1:B:139:PRO:HB3	1.87	0.56
1:B:157:MET:HE1	1:B:310:LEU:HD21	1.88	0.56
1:A:154:HIS:HE1	1:A:220:GLU:CD	2.14	0.56
1:A:244:GLN:O	1:A:245:GLN:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:TYR:O	1:C:314:ASP:C	2.48	0.56
1:B:134:THR:O	1:B:137:ILE:HD13	2.05	0.56
1:A:157:MET:HE1	1:A:314:ASP:OD1	2.06	0.56
1:B:126:LYS:HG2	1:C:299:THR:CG2	2.36	0.56
1:B:314:ASP:O	1:B:318:ILE:CG1	2.43	0.56
1:C:61:PHE:CE2	1:C:64:LEU:HG	2.41	0.56
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:107:ILE:HD12	1:B:128:VAL:HG11	1.87	0.55
1:B:238:TRP:HZ2	1:B:272:VAL:HG21	1.71	0.55
1:C:98:ILE:HD13	1:C:124:ASN:ND2	2.18	0.55
1:C:143:ALA:HB2	1:C:236:TYR:OH	2.06	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:B:254:VAL:C	1:B:256:GLU:H	2.14	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:B:67:MET:HE1	1:B:165:TYR:CB	2.37	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:C:173:PHE:O	1:C:174:VAL:C	2.50	0.55
1:A:198:ILE:HA	1:A:201:GLN:HB3	1.89	0.55
1:A:203:GLY:CA	1:C:301:GLU:OE2	2.51	0.55
1:B:220:GLU:OE2	1:B:241:ASN:OD1	2.25	0.55
1:B:244:GLN:O	1:B:245:GLN:HB2	2.06	0.55
1:A:61:PHE:CE1	1:A:63:VAL:HB	2.42	0.55
1:A:259:LYS:C	1:A:261:ASN:N	2.62	0.55
1:C:204:ALA:HA	1:C:207:GLU:CD	2.33	0.55
1:B:84:ILE:HG22	1:B:84:ILE:O	2.07	0.54
1:C:183:TYR:O	1:C:184:TYR:C	2.50	0.54
1:A:163:LEU:O	1:A:166:VAL:HG22	2.07	0.54
1:B:159:PRO:HB3	1:B:199:ASP:HB2	1.88	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:N	1:C:161:ASN:HD22	2.05	0.54
1:C:210:PRO:HG2	1:C:213:GLN:CD	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ILE:CG2	1:C:85:GLY:N	2.69	0.54
1:B:284:THR:C	1:B:286:ALA:H	2.16	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:A:248:PRO:HA	1:A:251:VAL:HG13	1.89	0.54
1:B:265:THR:HG21	1:B:267:PHE:HZ	1.69	0.54
1:C:98:ILE:CG1	1:C:121:PHE:CE1	2.90	0.54
1:C:106:LEU:HD22	1:C:176:LEU:HD22	1.90	0.54
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:A:114:LEU:HD13	1:A:153:PRO:HB2	1.89	0.54
1:B:213:GLN:HA	1:B:215:PHE:CD1	2.27	0.54
1:B:227:ALA:HA	1:B:232:MET:HB2	1.90	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:C:279:GLN:O	1:C:281:ALA:C	2.51	0.54
1:C:98:ILE:HG13	1:C:121:PHE:CE1	2.42	0.53
1:C:125:VAL:O	1:C:127:ASP:CA	2.56	0.53
1:A:106:LEU:HD12	1:A:107:ILE:H	1.73	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:194:GLN:NE2	1:B:135:GLU:HA	2.23	0.53
1:B:124:ASN:HA	1:C:84:ILE:HG21	1.90	0.53
1:B:167:GLU:HA	1:B:167:GLU:OE1	2.08	0.53
1:B:282:GLN:HG3	1:B:283:ALA:N	2.23	0.53
1:C:209:VAL:HG12	1:C:323:LEU:HD11	1.89	0.53
1:C:209:VAL:HG12	1:C:323:LEU:CD1	2.38	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:A:158:SER:HB2	1:A:225:TYR:HB3	1.91	0.53
1:B:319:THR:HG22	1:B:320:ASN:N	2.22	0.53
1:C:278:LYS:C	1:C:281:ALA:H	2.16	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:B:260:THR:HG23	1:B:261:ASN:HD22	1.73	0.53
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:A:182:LYS:HE3	1:A:183:TYR:CE1	2.45	0.52
1:B:307:PHE:O	1:B:310:LEU:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ALA:O	1:C:182:LYS:C	2.53	0.52
1:C:279:GLN:O	1:C:280:VAL:C	2.51	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:A:51:THR:O	1:A:52:GLU:C	2.51	0.52
1:A:67:MET:HE1	1:A:165:TYR:CB	2.39	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:A:98:ILE:O	1:A:102:GLN:HG2	2.10	0.51
1:B:88:ILE:HG13	1:B:89:HIS:N	2.25	0.51
1:B:126:LYS:O	1:B:127:ASP:O	2.28	0.51
1:B:156:TRP:C	1:B:158:SER:H	2.17	0.51
1:C:162:ALA:O	1:C:166:VAL:HG13	2.09	0.51
1:B:159:PRO:HB2	1:B:199:ASP:HB2	1.92	0.51
1:C:279:GLN:C	1:C:281:ALA:H	2.18	0.51
1:A:204:ALA:HA	1:A:207:GLU:OE1	2.10	0.51
1:B:258:VAL:HG13	1:B:263:VAL:O	2.11	0.51
1:C:106:LEU:HD11	1:C:131:VAL:CG1	2.39	0.51
1:C:182:LYS:O	1:C:183:TYR:C	2.53	0.51
1:A:246:PHE:CD1	1:A:246:PHE:C	2.88	0.51
1:A:219:CYS:HB3	1:A:238:TRP:CH2	2.46	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:C:110:ASN:O	1:C:134:THR:HB	2.10	0.51
1:C:254:VAL:CG1	1:C:280:VAL:HG21	2.41	0.51
1:A:125:VAL:O	1:A:125:VAL:HG23	2.11	0.51
1:A:200:ARG:HG3	1:C:301:GLU:HB3	1.93	0.51
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:126:LYS:HA	1:C:299:THR:HG21	1.94	0.50
1:B:265:THR:CG2	1:B:267:PHE:CE1	2.93	0.50
1:B:281:ALA:O	1:B:284:THR:O	2.28	0.50
1:B:317:VAL:O	1:B:320:ASN:O	2.30	0.50
1:C:246:PHE:O	1:C:246:PHE:CD1	2.65	0.50
1:B:320:ASN:O	1:B:320:ASN:OD1	2.30	0.50
1:C:198:ILE:O	1:C:202:LEU:HD13	2.11	0.50
1:A:94:THR:O	1:A:97:ASP:HB2	2.12	0.50
1:B:218:SER:HA	1:B:267:PHE:O	2.11	0.50
1:B:257:GLU:O	1:B:258:VAL:C	2.55	0.50
1:C:143:ALA:CB	1:C:236:TYR:OH	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:VAL:HG13	1:C:310:LEU:HB2	1.92	0.50
1:A:132:VAL:C	1:A:134:THR:H	2.20	0.50
1:A:312:GLU:OE1	4:A:332:CAC:O2	2.29	0.50
1:B:126:LYS:CG	1:C:299:THR:HG23	2.41	0.50
1:B:128:VAL:O	1:B:129:PRO:O	2.30	0.50
1:B:206:LEU:O	1:B:209:VAL:CG1	2.60	0.50
1:C:246:PHE:CE2	1:C:276:GLY:CA	2.93	0.50
1:A:276:GLY:O	1:A:279:GLN:HB2	2.11	0.50
1:B:266:ILE:HD13	1:B:280:VAL:CG2	2.41	0.50
1:C:281:ALA:O	1:C:282:GLN:CB	2.60	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:244:GLN:C	1:B:246:PHE:H	2.18	0.49
1:A:244:GLN:O	1:A:245:GLN:O	2.30	0.49
1:B:112:MET:HG3	1:B:134:THR:HG21	1.94	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:A:182:LYS:HE3	1:A:183:TYR:HE1	1.77	0.49
1:A:210:PRO:HG2	1:A:213:GLN:CD	2.37	0.49
1:A:293:TYR:O	1:A:310:LEU:HD11	2.13	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: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:179:ASP:OD1	4:A:2327:CAC:C1	2.61	0.49
1:A:260:THR:O	1:A:261:ASN:OD1	2.30	0.49
1:C:84:ILE:O	1:C:85:GLY:C	2.56	0.49
1:C:173:PHE:C	1:C:175:GLU:N	2.69	0.49
1:A:166:VAL:HA	1:A:169:ILE:HD12	1.95	0.48
1:B:108:LEU:HG	1:B:133:LEU:HD21	1.95	0.48
1:C:217:VAL:HG21	1:C:266:ILE:CB	2.43	0.48
1:C:220:GLU:OE1	1:C:222:ALA:HB2	2.13	0.48
1:A:68:VAL:CG2	1:A:78:VAL:HG11	2.43	0.48
1:A:304:VAL:HG13	1:A:310:LEU:CA	2.43	0.48
1:B:125:VAL:O	1:B:126:LYS:O	2.30	0.48
1:A:122:LEU:O	1:A:125:VAL:HG22	2.13	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: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:A:58:LEU:CD2	1:A:81:ILE:HD11	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:HG2	1:A:232:MET:HE3	1.95	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:C:220:GLU:CD	1:C:222:ALA:HB2	2.39	0.48
1:C:147:TYR:N	1:C:147:TYR:HD1	2.10	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:317:VAL:HG22	1:B:318:ILE:N	2.29	0.48
1:B:56:LYS:HG3	1:B:77:VAL:CG1	2.43	0.48
1:B:68:VAL:HG12	1:B:169:ILE:CD1	2.43	0.48
1:B:197:ALA:HA	1:B:200:ARG:HH21	1.79	0.48
1:A:266:ILE:HD11	1:A:281:ALA:HB2	1.95	0.48
1:C:114:LEU:HB2	1:C:153:PRO:HB2	1.96	0.48
1:B:58:LEU:HD21	1:B:81:ILE:CD1	2.43	0.47
1:B:200:ARG:O	1:B:201:GLN:C	2.57	0.47
1:B:217:VAL:CG1	1:B:266:ILE:HG22	2.44	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:A:304:VAL:HG13	1:A:310:LEU:HB2	1.96	0.47
1:C:245:GLN:O	1:C:246:PHE:O	2.33	0.47
1:A:190:VAL:HG21	1:B:139:PRO:HG3	1.97	0.47
1:B:121:PHE:O	1:B:125:VAL:CG1	2.62	0.47
1:C:177:ASP:CG	1:C:180:ASN:HD22	2.22	0.47
1:C:200:ARG:HB3	1:C:200:ARG:HH21	1.80	0.47
1:C:223:PHE:O	1:C:224:SER:C	2.57	0.47
1:B:140:ILE:HG12	1:B:225:TYR:CE1	2.50	0.47
1:A:110:ASN:C	1:A:110:ASN:HD22	2.23	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:B:304:VAL:HG12	1:B:304:VAL:O	2.15	0.47
1:C:276:GLY:O	1:C:279:GLN:HB2	2.15	0.47
1:B:88:ILE:HD12	1:B:114:LEU:HD21	1.95	0.46
1:C:278:LYS:O	1:C:279:GLN:C	2.57	0.46
1:A:198:ILE:O	1:A:202:LEU:HB2	2.15	0.46
1:A:269:GLU:HG2	1:A:294:VAL:CG2	2.45	0.46
1:C:142:ILE:CG2	1:C:143:ALA:H	2.15	0.46
1:C:266:ILE:CD1	1:C:277:GLN:HG3	2.45	0.46
1:B:198:ILE:HD11	1:B:311:LEU:CD1	2.42	0.46
1:B:219:CYS:O	1:B:238:TRP:CD2	2.68	0.46
1:B:182:LYS:HG2	1:B:183:TYR:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PRO:HG2	1:B:322:LEU:HA	1.96	0.46
1:C:121:PHE:C	1:C:123:GLY:N	2.71	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:250:GLN:C	1:C:252:GLN:N	2.73	0.46
1:B:310:LEU:C	1:B:310:LEU:HD23	2.41	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
1:A:87:GLU:OE1	1:A:89:HIS:HB2	2.16	0.46
1:B:323:LEU:N	1:B:323:LEU:CD1	2.78	0.46
1:B:238:TRP:CZ2	1:B:272:VAL:HG21	2.51	0.46
1:B:244:GLN:C	1:B:246:PHE:N	2.74	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:C:158:SER:O	1:C:161:ASN:N	2.49	0.45
1:A:83:ARG:HH11	1:A:100:LYS:NZ	2.14	0.45
1:B:254:VAL:C	1:B:256:GLU:N	2.73	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:118:PHE:O	1:A:119:GLU:C	2.59	0.45
1:B:84:ILE:O	1:B:84:ILE:CG2	2.58	0.45
1:C:218:SER:OG	1:C:269:GLU:OE2	2.33	0.45
1:A:64:LEU:HD13	1:A:133:LEU:HD12	1.97	0.45
1:A:190:VAL:HG22	1:B:112:MET:HG2	1.97	0.45
1:A:320:ASN:C	1:A:320:ASN:ND2	2.74	0.45
1:B:201:GLN:OE1	1:B:316:ARG:NH1	2.45	0.45
1:A:68:VAL:HG23	1:A:78:VAL:HG11	1.99	0.45
1:B:158:SER:O	1:B:161:ASN:HB2	2.17	0.45
1:C:77:VAL:O	1:C:77:VAL:HG22	2.16	0.45
1:C:117:TRP:CD1	1:C:117:TRP:H	2.35	0.45
1:C:161:ASN:O	1:C:164:VAL:HG22	2.17	0.45
1:B:56:LYS:HE2	5:B:14:HOH:O	2.16	0.45
1:C:125:VAL:HB	1:C:128:VAL:HG23	1.98	0.45
1:A:259:LYS:O	1:A:260:THR:C	2.59	0.45
1:B:137:ILE:CD1	1:B:164:VAL:CG2	2.80	0.45
1:B:284:THR:O	1:B:286:ALA:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LEU:HD11	1:C:156:TRP:HH2	1.81	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:B:299:THR:O	1:B:300:GLU:C	2.60	0.44
1:A:220:GLU:C	1:A:222:ALA:H	2.24	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:67:MET:HE2	1:A:67:MET:HB3	1.84	0.44
1:A:195:LEU:HD13	1:A:308:LEU:HD11	1.99	0.44
1:A:277:GLN:HA	1:A:277:GLN:NE2	2.28	0.44
1:C:113:ASN:O	1:C:114:LEU:C	2.61	0.44
1:C:237:MET:SD	1:C:246:PHE:CD2	3.11	0.44
1:A:125:VAL:O	1:A:125:VAL:CG2	2.62	0.44
1:C:171:GLN:O	1:C:174:VAL:HG22	2.17	0.44
1:B:233:GLU:HG3	1:B:234:GLU:H	1.81	0.44
1:B:274:ASP:HB3	5:B:18:HOH:O	2.16	0.44
1:A:157:MET:HE2	1:A:294:VAL:HG13	1.98	0.44
1:C:217:VAL:HG21	1:C:266:ILE:HB	1.99	0.44
1:A:87:GLU:O	1:A:87:GLU:HG3	2.16	0.44
1:A:127:ASP:C	1:A:128:VAL:HG23	2.43	0.44
1:A:158:SER:O	1:A:161:ASN:N	2.50	0.44
1:A:132:VAL:HG23	1:A:134:THR:H	1.83	0.44
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:217:VAL:CG2	1:C:266:ILE:HB	2.48	0.43
1:B:273:SER:OG	1:B:275:LYS:HG3	2.18	0.43
1:C:298:SER:O	1:C:305:PRO:HA	2.18	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:B:101:ALA:HB2	1:B:121:PHE:CZ	2.53	0.43
1:B:157:MET:HE2	1:B:294:VAL:CG1	2.46	0.43
1:C:52:GLU:HG3	1:C:53:GLU:N	2.33	0.43
1:C:259:LYS:CG	1:C:284:THR:OG1	2.39	0.43
1:C:278:LYS:HA	1:C:281:ALA:CB	2.45	0.43
1:A:102:GLN:HG2	1:A:102:GLN:H	1.58	0.43
1:A:137:ILE:HD11	1:A:164:VAL:HG23	2.00	0.43
1:C:57:VAL:HG12	1:C:58:LEU:N	2.34	0.43
1:C:98:ILE:HG12	1:C:121:PHE:CD1	2.53	0.43
1:C:244:GLN:HB3	1:C:245:GLN:H	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PRO:HA	1:A:225:TYR:OH	2.17	0.43
1:B:267:PHE:HB3	1:B:292:LEU:HG	2.01	0.43
1:B:284:THR:HG23	1:B:286:ALA:CB	2.48	0.43
1:C:208:GLN:O	1:C:209:VAL:C	2.60	0.43
1:C:258:VAL:HG23	1:C:263:VAL:HB	2.01	0.43
1:A:88:ILE:HD12	1:A:114:LEU:HD21	2.00	0.43
1:A:311:LEU:O	1:A:312:GLU:C	2.62	0.43
1:B:89:HIS:NE2	1:B:220:GLU:OE2	2.52	0.43
1:B:282:GLN:HE21	1:B:282:GLN:HB2	1.63	0.43
1:A:307:PHE:CZ	1:A:311:LEU:HD11	2.54	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:213:GLN:O	1:C:322:LEU:HD13	2.18	0.43
1:B:58:LEU:HA	1:B:79:GLU:O	2.19	0.42
1:B:117:TRP:CD1	1:B:117:TRP:H	2.35	0.42
1:B:239:PRO:HG2	1:B:240:ILE:H	1.84	0.42
1:C:97:ASP:OD2	1:C:97:ASP:N	2.52	0.42
1:B:122:LEU:O	1:B:125:VAL:HG13	2.19	0.42
1:B:211:ALA:HA	1:B:214:ARG:NE	2.33	0.42
1:B:158:SER:O	1:B:161:ASN:N	2.48	0.42
1:B:267:PHE:CE2	1:B:317:VAL:CG2	3.02	0.42
1:C:304:VAL:O	1:C:304:VAL:HG12	2.19	0.42
1:A:140:ILE:HG12	1:A:225:TYR:CE1	2.55	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:112:MET:CG	1:A:134:THR:HG21	2.36	0.42
1:A:259:LYS:O	1:A:261:ASN:N	2.53	0.42
1:C:91:TYR:OH	1:C:97:ASP:OD1	2.36	0.42
1:C:201:GLN:HE21	1:C:312:GLU:HG3	1.82	0.42
1:A:147:TYR:O	1:A:148:THR:C	2.60	0.42
1:A:258:VAL:HG12	1:A:259:LYS:H	1.77	0.42
1:B:279:GLN:HA	1:B:282:GLN:HG2	2.02	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:101:ALA:HB2	1:A:121:PHE:CZ	2.55	0.42
1:B:245:GLN:OE1	1:B:245:GLN:HA	2.20	0.42
1:C:183:TYR:C	1:C:185:ASN:N	2.76	0.42
1:C:295:ASP:O	1:C:296:SER:CB	2.68	0.42
1:A:170:ARG:HG3	1:A:188:ALA:HB2	2.01	0.42
1:B:163:LEU:HA	1:B:163:LEU:HD23	1.79	0.42
1:B:218:SER:O	1:B:236:TYR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:HIS:CD2	1:A:222:ALA:HB1	2.54	0.42
1:A:220:GLU:C	1:A:222:ALA:N	2.77	0.42
1:B:255:ILE:HG13	1:B:255:ILE:H	1.70	0.42
1:A:77:VAL:O	1:A:77:VAL:HG22	2.20	0.41
1:A:137:ILE:HG12	1:A:164:VAL:CG2	2.33	0.41
1:B:148:THR:HG23	1:B:149:ASP:N	2.34	0.41
1:C:223:PHE:CE2	1:C:294:VAL:CG1	3.03	0.41
1:C:248:PRO:O	1:C:252:GLN:HB2	2.20	0.41
1:B:158:SER:O	1:B:159:PRO:C	2.63	0.41
1:C:64:LEU:HD13	1:C:133:LEU:HD12	2.02	0.41
1:A:98:ILE:HG21	1:A:124:ASN:HD21	1.78	0.41
1:A:147:TYR:HA	1:A:150:LYS:HG2	2.02	0.41
1:B:115:GLU:H	1:B:115:GLU:CD	2.28	0.41
1:B:118:PHE:O	1:B:119:GLU:C	2.63	0.41
1:C:244:GLN:C	1:C:245:GLN:CG	2.92	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:190:VAL:O	1:C:193:GLU:HB3	2.21	0.41
1:C:205:ASP:O	1:C:208:GLN:HG3	2.21	0.41
1:C:214:ARG:HG2	1:C:232:MET:HE3	2.02	0.41
1:A:110:ASN:C	1:A:110:ASN:ND2	2.79	0.41
1:A:127:ASP:O	1:A:128:VAL:HG23	2.20	0.41
1:A:180:ASN:O	1:A:181:ALA:C	2.64	0.41
1:B:257:GLU:C	1:B:260:THR:HG22	2.42	0.41
1:B:323:LEU:N	1:B:323:LEU:HD12	2.35	0.41
1:C:277:GLN:O	1:C:280:VAL:HB	2.21	0.41
1:A:191:TYR:HE1	1:A:308:LEU:HD22	1.86	0.41
1:A:226:LEU:HA	1:A:226:LEU:HD12	1.69	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:C:223:PHE:C	1:C:225:TYR:N	2.77	0.41
1:C:316:ARG:H	1:C:316:ARG:HG3	1.52	0.41
1:A:253:THR:O	1:A:256:GLU:HG2	2.21	0.41
1:B:152:ASN:O	1:B:225:TYR:OH	2.39	0.41
1:C:220:GLU:HB2	1:C:238:TRP:HE1	1.85	0.41
1:B:124:ASN:CB	1:C:84:ILE:HG22	2.51	0.40
1:B:258:VAL:O	1:B:262:ASN:CA	2.65	0.40
1:C:220:GLU:C	1:C:222:ALA:N	2.79	0.40
1:C:58:LEU:HD12	1:C:58:LEU:HA	1.84	0.40
1:C:128:VAL:HA	1:C:129:PRO:HD2	1.76	0.40
1:C:211:ALA:C	1:C:213:GLN:H	2.30	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	272/307 (89%)	233 (86%)	33 (12%)	6 (2%)	5	14
1	B	263/307 (86%)	222 (84%)	31 (12%)	10 (4%)	2	5
1	C	270/307 (88%)	215 (80%)	32 (12%)	23 (8%)	0	1
All	All	805/921 (87%)	670 (83%)	96 (12%)	39 (5%)	2	3

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	193 (82%)	41 (18%)	2	5
1	B	229/259 (88%)	176 (77%)	53 (23%)	1	2
1	C	233/259 (90%)	186 (80%)	47 (20%)	1	4
All	All	696/777 (90%)	555 (80%)	141 (20%)	1	3

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

Mol	Chain	Res	Type
1	A	52	GLU
1	A	56	LYS
1	A	77	VAL
1	A	84	ILE

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Mol	Chain	Res	Type
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	131	VAL
1	A	132	VAL
1	A	134	THR
1	A	138	GLU
1	A	148	THR
1	A	149	ASP
1	A	150	LYS
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	251	VAL
1	A	258	VAL
1	A	260	THR
1	A	268	CYS
1	A	280	VAL
1	A	284	THR
1	A	287	ARG
1	A	294	VAL
1	A	304	VAL
1	A	308	LEU
1	A	317	VAL
1	A	320	ASN
1	A	322	LEU
1	A	323	LEU
1	B	56	LYS
1	B	64	LEU
1	B	68	VAL
1	B	83	ARG
1	B	84	ILE

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Mol	Chain	Res	Type
1	B	87	GLU
1	B	96	SER
1	B	98	ILE
1	B	100	LYS
1	B	108	LEU
1	B	120	GLN
1	B	124	ASN
1	B	125	VAL
1	B	130	SER
1	B	131	VAL
1	B	132	VAL
1	B	134	THR
1	B	135	GLU
1	B	137	ILE
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	202	LEU
1	B	205	ASP
1	B	209	VAL
1	B	214	ARG
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	254	VAL
1	B	256	GLU
1	B	259	LYS
1	B	265	THR
1	B	277	GLN
1	B	280	VAL
1	B	282	GLN
1	B	287	ARG

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Mol	Chain	Res	Type
1	B	294	VAL
1	B	299	THR
1	B	308	LEU
1	B	317	VAL
1	B	318	ILE
1	B	319	THR
1	C	53	GLU
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	108	LEU
1	C	115	GLU
1	C	124	ASN
1	C	126	LYS
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	169	ILE
1	C	174	VAL
1	C	175	GLU
1	C	182	LYS
1	C	190	VAL
1	C	195	LEU
1	C	198	ILE
1	C	205	ASP
1	C	207	GLU
1	C	208	GLN
1	C	209	VAL
1	C	217	VAL
1	C	218	SER
1	C	220	GLU
1	C	240	ILE
1	C	243	GLU
1	C	245	GLN

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Mol	Chain	Res	Type
1	C	246	PHE
1	C	251	VAL
1	C	273	SER
1	C	277	GLN
1	C	279	GLN
1	C	284	THR
1	C	287	ARG
1	C	294	VAL
1	C	299	THR
1	C	316	ARG
1	C	317	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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	A	320	ASN
1	B	120	GLN
1	B	124	ASN
1	B	161	ASN
1	B	180	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	213	GLN
1	C	244	GLN
1	C	277	GLN

5.3.3 RNA ⓘ

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](#)

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	C	2327	-	2,4,4	12.10	2 (100%)	4,6,6	3.57	2 (50%)
4	CAC	A	2327	-	2,4,4	16.05	2 (100%)	4,6,6	6.61	3 (75%)
4	CAC	C	332	-	2,4,4	14.88	2 (100%)	4,6,6	9.27	3 (75%)
4	CAC	A	332	-	2,4,4	11.78	2 (100%)	4,6,6	5.81	4 (100%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2327	CAC	AS-C2	-17.76	1.48	1.90
4	C	332	CAC	AS-C2	-17.10	1.50	1.90
4	A	2327	CAC	AS-C1	-14.14	1.57	1.90
4	C	2327	CAC	AS-C2	-12.57	1.60	1.90
4	C	332	CAC	AS-C1	-12.27	1.61	1.90
4	A	332	CAC	AS-C1	-12.04	1.62	1.90
4	C	2327	CAC	AS-C1	-11.60	1.63	1.90
4	A	332	CAC	AS-C2	-11.50	1.63	1.90

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	332	CAC	O1-AS-C1	-17.05	90.30	111.50
4	A	2327	CAC	O1-AS-C1	-9.36	99.86	111.50
4	A	2327	CAC	O1-AS-C2	7.84	121.25	111.50
4	A	332	CAC	O1-AS-C1	7.62	120.97	111.50
4	C	332	CAC	O2-AS-C1	6.76	122.22	105.84
4	C	2327	CAC	O1-AS-C2	-5.53	104.62	111.50
4	A	332	CAC	O2-AS-C2	5.28	118.63	105.84
4	A	332	CAC	O2-AS-C1	5.11	118.21	105.84
4	A	2327	CAC	O2-AS-C1	5.02	117.99	105.84
4	A	332	CAC	O1-AS-C2	4.82	117.49	111.50
4	C	2327	CAC	O2-AS-C2	4.25	116.12	105.84
4	C	332	CAC	O1-AS-C2	2.30	114.36	111.50

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%)	-0.22	3 (1%) 78 76	59, 77, 102, 116	0
1	B	267/307 (86%)	-0.07	2 (0%) 84 83	54, 83, 120, 131	0
1	C	272/307 (88%)	0.04	4 (1%) 72 70	24, 95, 136, 162	0
All	All	813/921 (88%)	-0.08	9 (1%) 78 76	24, 83, 129, 162	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	126	LYS	3.9
1	A	244	GLN	3.1
1	C	127	ASP	3.0
1	B	128	VAL	3.0
1	C	125	VAL	2.6
1	A	242	ALA	2.6
1	C	280	VAL	2.6
1	A	324	ALA	2.3
1	B	254	VAL	2.3

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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	3	1/1	0.58	0.09	110,110,110,110	1
3	ZN	C	331	1/1	0.64	0.23	133,133,133,133	0
4	CAC	A	332	5/5	0.72	0.15	68,83,91,114	1
4	CAC	A	2327	5/5	0.76	0.09	133,134,149,199	0
4	CAC	C	2327	5/5	0.80	0.10	98,102,111,143	1
4	CAC	C	332	5/5	0.80	0.09	127,139,141,166	1
3	ZN	A	5	1/1	0.87	0.06	142,142,142,142	0
3	ZN	A	2	1/1	0.91	0.07	88,88,88,88	1
3	ZN	A	331	1/1	0.92	0.08	113,113,113,113	0
3	ZN	C	4	1/1	0.94	0.20	111,111,111,111	0
2	MN	A	1	1/1	0.99	0.07	56,56,56,56	0
2	MN	C	1	1/1	0.99	0.05	85,85,85,85	0
2	MN	B	1	1/1	1.00	0.04	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.