



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:53 AM UTC

PDB ID : 4EED / pdb_00004eed
Title : CorA coiled-coil mutant under Mg²⁺ presence
Authors : Pfoh, R.; Pai, E.F.
Deposited on : 2012-03-28
Resolution : 3.92 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
Xtrriage (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

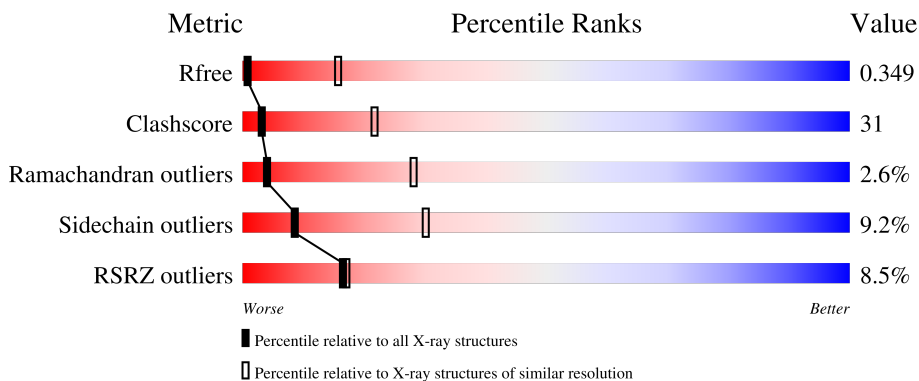
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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	330	 10% 44% 44% 6% • 5%
1	B	330	 5% 47% 44% • • 5%
1	C	330	 10% 47% 42% 6% • 5%
1	D	330	 8% 42% 45% 7% • 5%
1	E	330	 7% 45% 42% 8% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12979 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 Magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2593	1688	418	478	9	0	0	0
1	B	314	2593	1688	418	478	9	0	0	0
1	C	314	2593	1688	418	478	9	0	0	0
1	D	314	2593	1688	418	478	9	0	0	0
1	E	314	2593	1688	418	478	9	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q9WZ31
A	23	SER	-	expression tag	UNP Q9WZ31
A	24	HIS	-	expression tag	UNP Q9WZ31
A	25	MET	-	expression tag	UNP Q9WZ31
A	222	ALA	ARG	engineered mutation	UNP Q9WZ31
A	223	ALA	LYS	engineered mutation	UNP Q9WZ31
B	22	GLY	-	expression tag	UNP Q9WZ31
B	23	SER	-	expression tag	UNP Q9WZ31
B	24	HIS	-	expression tag	UNP Q9WZ31
B	25	MET	-	expression tag	UNP Q9WZ31
B	222	ALA	ARG	engineered mutation	UNP Q9WZ31
B	223	ALA	LYS	engineered mutation	UNP Q9WZ31
C	22	GLY	-	expression tag	UNP Q9WZ31
C	23	SER	-	expression tag	UNP Q9WZ31
C	24	HIS	-	expression tag	UNP Q9WZ31
C	25	MET	-	expression tag	UNP Q9WZ31
C	222	ALA	ARG	engineered mutation	UNP Q9WZ31
C	223	ALA	LYS	engineered mutation	UNP Q9WZ31
D	22	GLY	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	23	SER	-	expression tag	UNP Q9WZ31
D	24	HIS	-	expression tag	UNP Q9WZ31
D	25	MET	-	expression tag	UNP Q9WZ31
D	222	ALA	ARG	engineered mutation	UNP Q9WZ31
D	223	ALA	LYS	engineered mutation	UNP Q9WZ31
E	22	GLY	-	expression tag	UNP Q9WZ31
E	23	SER	-	expression tag	UNP Q9WZ31
E	24	HIS	-	expression tag	UNP Q9WZ31
E	25	MET	-	expression tag	UNP Q9WZ31
E	222	ALA	ARG	engineered mutation	UNP Q9WZ31
E	223	ALA	LYS	engineered mutation	UNP Q9WZ31

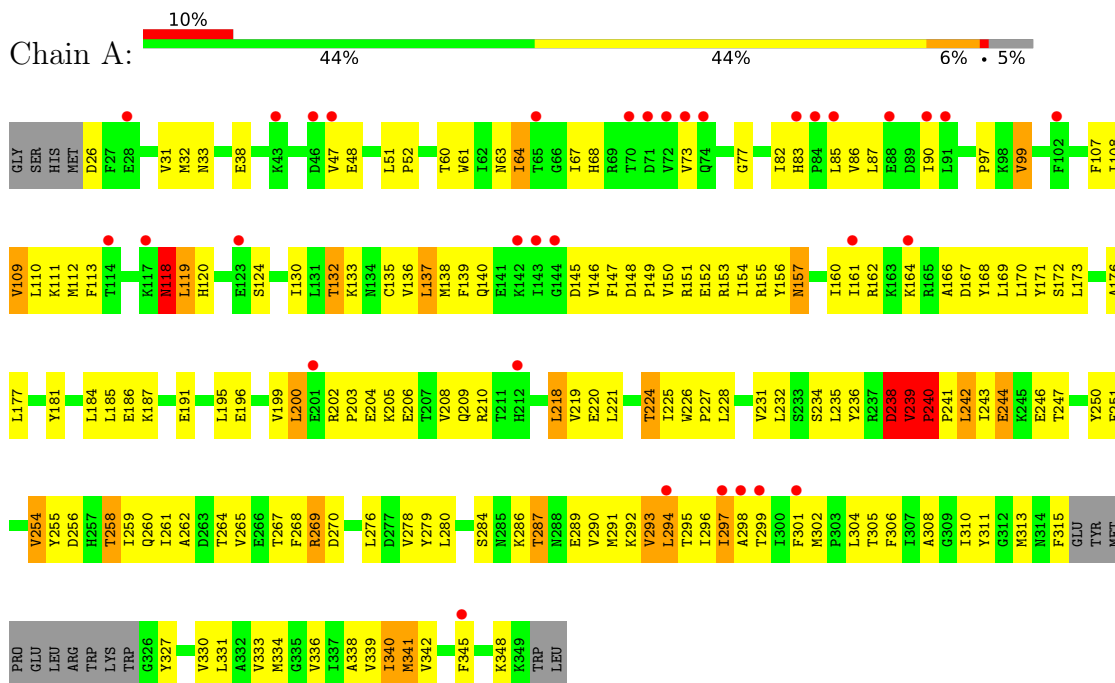
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	3	Total Mg 3 3	0	0
2	C	2	Total Mg 2 2	0	0
2	D	3	Total Mg 3 3	0	0
2	E	2	Total Mg 2 2	0	0

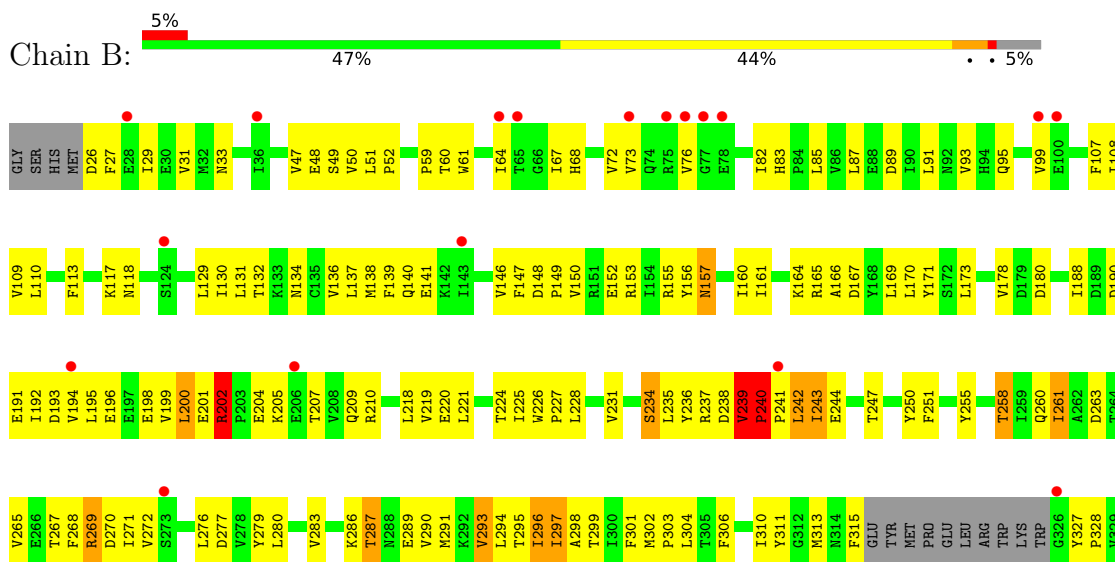
3 Residue-property plots

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: Magnesium transport protein CorA

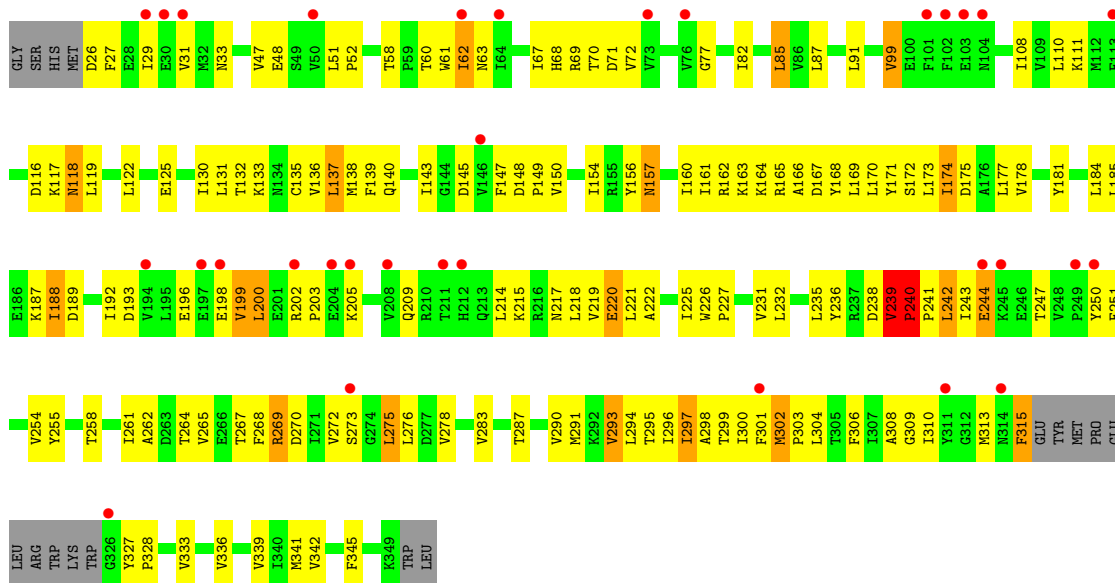


- Molecule 1: Magnesium transport protein CorA

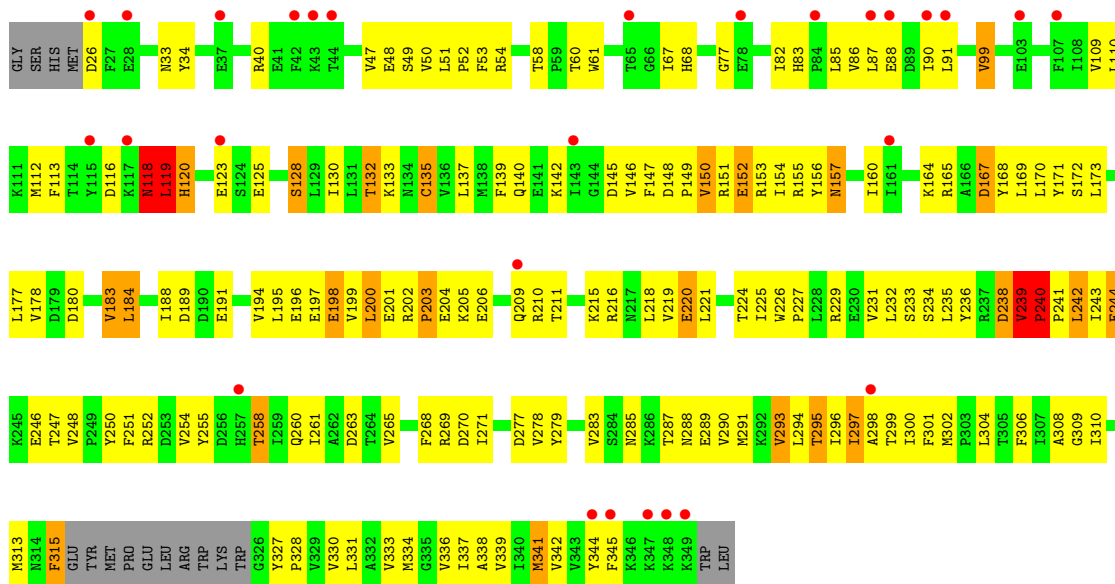




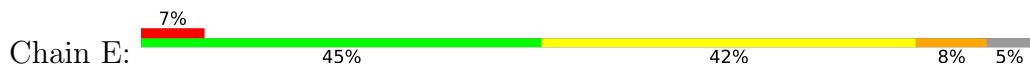
• Molecule 1: Magnesium transport protein CorA



• Molecule 1: Magnesium transport protein CorA



• Molecule 1: Magnesium transport protein CorA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.70Å 132.50Å 179.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.92 48.79 – 3.92	Depositor EDS
% Data completeness (in resolution range)	82.1 (48.79-3.92) 81.9 (48.79-3.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.88Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.297 , 0.351 0.297 , 0.349	Depositor DCC
R_{free} test set	1097 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	142.1	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 137.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12979	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.73	2/2646 (0.1%)	0.88	3/3588 (0.1%)
1	B	0.70	1/2646 (0.0%)	0.85	1/3588 (0.0%)
1	C	0.71	1/2646 (0.0%)	0.86	3/3588 (0.1%)
1	D	0.78	3/2646 (0.1%)	0.90	2/3588 (0.1%)
1	E	0.73	0/2646	0.90	1/3588 (0.0%)
All	All	0.73	7/13230 (0.1%)	0.88	10/17940 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	ASP	CA-C	6.96	1.55	1.52
1	D	240	PRO	CA-C	5.95	1.57	1.52
1	C	143	ILE	CA-CB	5.63	1.59	1.54
1	D	271	ILE	CA-CB	-5.63	1.47	1.54
1	A	240	PRO	CA-C	5.31	1.57	1.52
1	D	238	ASP	CA-C	5.20	1.54	1.52
1	B	240	PRO	CA-C	5.01	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	VAL	CB-CA-C	-6.58	103.42	112.04
1	E	254	VAL	N-CA-C	-6.04	105.93	111.67
1	A	64	ILE	CB-CA-C	-5.75	105.32	112.45
1	B	272	VAL	CB-CA-C	-5.74	104.30	112.22
1	D	240	PRO	N-CA-C	5.35	117.23	110.70
1	A	240	PRO	N-CA-C	5.32	117.18	110.70
1	D	167	ASP	N-CA-C	-5.23	105.48	111.07
1	A	254	VAL	N-CA-C	-5.19	106.74	111.67
1	C	240	PRO	N-CA-C	5.10	116.92	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	VAL	CB-CA-C	-5.09	105.37	112.04

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	2593	0	2630	193	0
1	B	2593	0	2630	165	0
1	C	2593	0	2630	172	0
1	D	2593	0	2630	178	0
1	E	2593	0	2630	176	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
All	All	12979	0	13150	816	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 31.

All (816) 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:221:LEU:HG	1:B:225:ILE:HD11	1.27	1.17
1:C:294:LEU:HD22	1:D:294:LEU:HD11	1.11	1.05
1:E:221:LEU:HG	1:E:225:ILE:HD11	1.36	1.04
1:B:302:MET:HE3	1:C:301:PHE:HB2	1.39	1.04
1:B:302:MET:HE2	1:C:298:ALA:HA	1.40	1.02
1:C:99:VAL:HG21	1:C:235:LEU:HD13	1.42	0.99
1:D:33:ASN:CG	1:D:60:THR:HG22	1.86	0.98
1:A:276:LEU:HD23	1:E:277:ASP:HB3	1.51	0.93
1:B:255:TYR:O	1:B:258:THR:HG22	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:TYR:O	1:C:258:THR:HG22	1.68	0.93
1:C:70:THR:HG22	1:C:91:LEU:HD22	1.51	0.92
1:C:310:ILE:O	1:C:313:MET:HG2	1.71	0.91
1:A:310:ILE:O	1:A:313:MET:HG2	1.70	0.90
1:D:339:VAL:HA	1:D:342:VAL:HG12	1.54	0.90
1:D:255:TYR:O	1:D:258:THR:HG22	1.75	0.87
1:A:221:LEU:CD1	1:A:225:ILE:HD11	2.05	0.86
1:A:255:TYR:O	1:A:258:THR:HG22	1.76	0.86
1:B:294:LEU:HD22	1:C:294:LEU:CD1	2.07	0.85
1:E:211:THR:HG21	1:E:276:LEU:HD13	1.58	0.84
1:D:221:LEU:HG	1:D:225:ILE:HD11	1.60	0.83
1:E:67:ILE:HG22	1:E:91:LEU:HD23	1.60	0.83
1:B:310:ILE:O	1:B:313:MET:HG2	1.79	0.82
1:B:294:LEU:C	1:B:294:LEU:HD23	2.05	0.82
1:B:294:LEU:CD2	1:C:294:LEU:HD11	2.09	0.82
1:E:296:ILE:HG22	1:E:345:PHE:CE2	2.16	0.81
1:A:111:LYS:O	1:A:181:TYR:OH	1.97	0.81
1:B:291:MET:CE	1:C:290:VAL:HG12	2.11	0.81
1:E:221:LEU:CG	1:E:225:ILE:HD11	2.10	0.80
1:B:294:LEU:HD22	1:C:294:LEU:HD12	1.63	0.80
1:E:197:GLU:HA	1:E:200:LEU:HD22	1.64	0.80
1:B:236:TYR:HA	1:B:251:PHE:HZ	1.46	0.80
1:A:298:ALA:HA	1:E:302:MET:HE2	1.64	0.80
1:C:221:LEU:HG	1:C:225:ILE:HD11	1.62	0.80
1:E:255:TYR:O	1:E:258:THR:HG22	1.82	0.79
1:D:152:GLU:OE2	1:D:155:ARG:HD2	1.82	0.79
1:D:310:ILE:O	1:D:313:MET:HG2	1.83	0.78
1:C:339:VAL:HA	1:C:342:VAL:HG12	1.64	0.78
1:E:236:TYR:HA	1:E:251:PHE:HZ	1.47	0.78
1:A:302:MET:HE2	1:B:298:ALA:HA	1.65	0.78
1:B:47:VAL:HG23	1:B:72:VAL:HG13	1.66	0.78
1:A:99:VAL:HB	1:A:231:VAL:HG13	1.67	0.77
1:E:147:PHE:O	1:E:150:VAL:HG12	1.83	0.77
1:A:108:ILE:HD11	1:A:235:LEU:HD21	1.67	0.77
1:B:61:TRP:HB2	1:B:169:LEU:HD21	1.67	0.77
1:C:296:ILE:HG22	1:C:345:PHE:CE2	2.19	0.77
1:E:221:LEU:O	1:E:225:ILE:HD12	1.85	0.76
1:B:258:THR:HA	1:B:261:ILE:HD12	1.68	0.76
1:A:308:ALA:O	1:E:313:MET:HE1	1.85	0.76
1:A:73:VAL:HG12	1:A:87:LEU:HD22	1.68	0.76
1:B:294:LEU:HD21	1:C:294:LEU:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HG22	1:A:262:ALA:HB2	1.66	0.75
1:D:302:MET:CE	1:E:298:ALA:HA	2.16	0.75
1:D:330:VAL:HG13	1:D:331:LEU:HD12	1.68	0.75
1:E:327:TYR:O	1:E:330:VAL:HG12	1.86	0.75
1:D:236:TYR:HA	1:D:251:PHE:HZ	1.50	0.75
1:D:147:PHE:O	1:D:150:VAL:HG12	1.87	0.75
1:C:236:TYR:HA	1:C:251:PHE:HZ	1.53	0.74
1:A:90:ILE:HD11	1:A:130:ILE:HD11	1.68	0.74
1:C:131:LEU:HD13	1:C:136:VAL:HG22	1.68	0.73
1:C:315:PHE:CZ	1:D:327:TYR:HA	2.23	0.73
1:C:26:ASP:O	1:C:68:HIS:NE2	2.20	0.73
1:E:330:VAL:HG13	1:E:331:LEU:HD12	1.68	0.73
1:E:299:THR:HG21	1:E:345:PHE:CE2	2.24	0.73
1:A:299:THR:HG21	1:A:345:PHE:CZ	2.24	0.72
1:B:73:VAL:HG12	1:B:87:LEU:HD22	1.70	0.72
1:C:147:PHE:O	1:C:150:VAL:HG12	1.88	0.72
1:A:110:LEU:HD13	1:A:177:LEU:HD22	1.70	0.72
1:E:109:VAL:O	1:E:110:LEU:HD23	1.88	0.72
1:A:239:VAL:HB	1:A:242:LEU:HD23	1.72	0.72
1:D:295:THR:HG23	1:E:294:LEU:HB2	1.71	0.72
1:B:339:VAL:HA	1:B:342:VAL:HG12	1.72	0.72
1:E:67:ILE:HG22	1:E:67:ILE:O	1.90	0.72
1:A:150:VAL:HG11	1:A:173:LEU:HD23	1.72	0.71
1:A:199:VAL:HG11	1:A:278:VAL:HB	1.72	0.71
1:A:112:MET:CE	1:A:146:VAL:HG13	2.21	0.71
1:C:154:ILE:HG12	1:C:161:ILE:HG21	1.71	0.71
1:E:299:THR:HG21	1:E:345:PHE:CZ	2.26	0.71
1:E:296:ILE:HA	1:E:299:THR:HG22	1.74	0.70
1:C:238:ASP:C	1:C:239:VAL:HG23	2.17	0.70
1:C:165:ARG:HD3	1:C:243:ILE:HD11	1.73	0.69
1:B:294:LEU:CD2	1:C:294:LEU:CD1	2.69	0.69
1:C:48:GLU:HA	1:C:51:LEU:HD13	1.75	0.69
1:A:333:VAL:O	1:A:336:VAL:HG12	1.93	0.69
1:C:294:LEU:HD22	1:D:294:LEU:CD1	2.05	0.68
1:D:239:VAL:HB	1:D:242:LEU:HD23	1.76	0.68
1:A:208:VAL:HG12	1:E:278:VAL:HG13	1.74	0.68
1:A:118:ASN:O	1:A:120:HIS:N	2.26	0.68
1:C:296:ILE:CD1	1:C:297:ILE:HD12	2.23	0.68
1:A:225:ILE:HG21	1:A:261:ILE:HG22	1.76	0.68
1:D:118:ASN:O	1:D:120:HIS:N	2.27	0.68
1:E:310:ILE:O	1:E:313:MET:HG2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:HA	1:B:276:LEU:HD21	1.76	0.68
1:D:67:ILE:HG22	1:D:67:ILE:O	1.92	0.68
1:D:232:LEU:CD2	1:D:254:VAL:HG12	2.23	0.67
1:A:301:PHE:HB2	1:E:302:MET:HE3	1.77	0.67
1:B:296:ILE:CD1	1:B:297:ILE:HD12	2.23	0.67
1:A:82:ILE:HD13	1:A:130:ILE:HD13	1.76	0.67
1:A:264:THR:O	1:A:265:VAL:C	2.34	0.67
1:E:160:ILE:HG22	1:E:160:ILE:O	1.95	0.67
1:E:177:LEU:C	1:E:177:LEU:HD23	2.20	0.67
1:D:293:VAL:HG12	1:D:294:LEU:N	2.10	0.67
1:D:296:ILE:HD11	1:D:297:ILE:HD12	1.75	0.67
1:C:67:ILE:HG22	1:C:91:LEU:HD23	1.76	0.67
1:E:150:VAL:HG11	1:E:173:LEU:HD23	1.76	0.67
1:E:267:THR:O	1:E:271:ILE:HD12	1.95	0.67
1:A:147:PHE:O	1:A:150:VAL:HG12	1.96	0.66
1:B:31:VAL:HG21	1:B:50:VAL:HG12	1.77	0.66
1:A:290:VAL:HG12	1:E:291:MET:CE	2.25	0.66
1:D:177:LEU:C	1:D:177:LEU:HD23	2.20	0.66
1:E:307:ILE:HA	1:E:310:ILE:HD12	1.77	0.66
1:A:206:GLU:HB2	1:A:209:GLN:HG2	1.76	0.66
1:E:267:THR:HG22	1:E:271:ILE:HD11	1.78	0.66
1:B:67:ILE:HG22	1:B:67:ILE:O	1.94	0.65
1:B:107:PHE:CZ	1:B:109:VAL:HG22	2.30	0.65
1:A:99:VAL:HG21	1:A:235:LEU:HD13	1.77	0.65
1:A:304:LEU:HD11	1:A:338:ALA:HB2	1.79	0.65
1:C:85:LEU:HD23	1:C:85:LEU:H	1.62	0.65
1:E:330:VAL:O	1:E:333:VAL:HG12	1.96	0.65
1:B:221:LEU:HG	1:B:225:ILE:CD1	2.15	0.65
1:A:221:LEU:HD12	1:A:225:ILE:HD11	1.79	0.65
1:C:196:GLU:O	1:C:200:LEU:HD22	1.97	0.65
1:A:236:TYR:HA	1:A:251:PHE:HZ	1.62	0.65
1:C:221:LEU:HG	1:C:225:ILE:CD1	2.27	0.64
1:E:64:ILE:HD12	1:E:139:PHE:CE1	2.32	0.64
1:A:290:VAL:HG12	1:E:291:MET:HE3	1.80	0.64
1:B:295:THR:HG21	1:C:293:VAL:HG12	1.80	0.64
1:B:330:VAL:HA	1:B:333:VAL:HG12	1.79	0.64
1:D:191:GLU:HG3	1:D:195:LEU:HD22	1.80	0.64
1:D:331:LEU:HA	1:D:334:MET:HE3	1.78	0.64
1:A:196:GLU:O	1:A:200:LEU:HD22	1.96	0.64
1:B:178:VAL:HG13	1:B:261:ILE:HD11	1.78	0.64
1:C:77:GLY:HA2	1:C:82:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ASN:CG	1:D:60:THR:CG2	2.69	0.64
1:A:67:ILE:O	1:A:67:ILE:HG22	1.96	0.64
1:A:82:ILE:CD1	1:A:130:ILE:HD13	2.27	0.64
1:D:296:ILE:CD1	1:D:297:ILE:HD12	2.28	0.64
1:D:225:ILE:HG21	1:D:261:ILE:HG22	1.79	0.64
1:B:296:ILE:HD12	1:B:297:ILE:HD12	1.80	0.63
1:C:177:LEU:C	1:C:177:LEU:HD23	2.24	0.63
1:C:77:GLY:HA3	1:C:87:LEU:HD21	1.80	0.63
1:D:112:MET:CE	1:D:146:VAL:HG13	2.28	0.63
1:C:225:ILE:HG22	1:C:262:ALA:HB2	1.81	0.63
1:D:199:VAL:HG13	1:D:279:TYR:HA	1.81	0.63
1:A:160:ILE:O	1:A:160:ILE:HG22	1.98	0.63
1:A:208:VAL:CG1	1:E:278:VAL:HG13	2.29	0.62
1:B:302:MET:HE3	1:C:301:PHE:CB	2.21	0.62
1:B:196:GLU:O	1:B:200:LEU:HD22	1.98	0.62
1:E:67:ILE:CG2	1:E:91:LEU:HD23	2.30	0.62
1:A:306:PHE:CE1	1:B:304:LEU:HB3	2.34	0.62
1:A:77:GLY:HA3	1:A:87:LEU:HD21	1.82	0.62
1:B:296:ILE:HA	1:B:299:THR:HG22	1.80	0.62
1:D:48:GLU:HA	1:D:51:LEU:HD13	1.81	0.62
1:A:225:ILE:CG2	1:A:262:ALA:HB2	2.30	0.62
1:D:99:VAL:HB	1:D:231:VAL:HG13	1.81	0.61
1:A:199:VAL:HG13	1:A:279:TYR:HA	1.82	0.61
1:C:296:ILE:HG22	1:C:345:PHE:CD2	2.34	0.61
1:A:293:VAL:O	1:A:296:ILE:HG13	2.01	0.61
1:B:310:ILE:HG22	1:B:311:TYR:HD1	1.65	0.61
1:A:270:ASP:OD2	1:B:269:ARG:NH1	2.34	0.61
1:A:299:THR:HG21	1:A:345:PHE:CE2	2.35	0.60
1:B:296:ILE:O	1:B:299:THR:HG22	2.01	0.60
1:D:112:MET:HE3	1:D:146:VAL:HG13	1.82	0.60
1:D:294:LEU:HD22	1:E:294:LEU:HD11	1.83	0.60
1:E:99:VAL:HB	1:E:231:VAL:HG13	1.83	0.60
1:C:313:MET:HE1	1:D:308:ALA:O	2.02	0.60
1:D:171:TYR:O	1:D:250:TYR:CE2	2.54	0.60
1:A:112:MET:HE1	1:A:146:VAL:HG22	1.84	0.60
1:D:116:ASP:OD1	1:D:119:LEU:HB3	2.01	0.60
1:E:171:TYR:CD1	1:E:251:PHE:HB3	2.36	0.60
1:A:238:ASP:C	1:A:239:VAL:HG23	2.26	0.60
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.83	0.60
1:C:47:VAL:HG13	1:C:48:GLU:HG2	1.84	0.60
1:D:167:ASP:OD1	1:D:168:TYR:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ILE:HD13	1:B:218:LEU:HD11	1.84	0.59
1:E:232:LEU:CD2	1:E:254:VAL:HG12	2.32	0.59
1:C:48:GLU:OE1	1:C:51:LEU:HD22	2.02	0.59
1:D:33:ASN:CB	1:D:60:THR:HG22	2.32	0.59
1:A:130:ILE:HD12	1:A:139:PHE:HE2	1.67	0.59
1:D:61:TRP:HB2	1:D:169:LEU:HD21	1.85	0.59
1:E:82:ILE:HD13	1:E:130:ILE:HD13	1.83	0.59
1:D:77:GLY:HA3	1:D:87:LEU:HD21	1.85	0.59
1:D:296:ILE:HD12	1:D:297:ILE:N	2.18	0.59
1:E:238:ASP:C	1:E:239:VAL:HG23	2.26	0.59
1:A:137:LEU:HD22	1:A:139:PHE:CE2	2.38	0.59
1:C:160:ILE:HG22	1:C:160:ILE:O	2.03	0.59
1:D:171:TYR:CD1	1:D:251:PHE:HB3	2.37	0.59
1:E:160:ILE:HG23	1:E:163:LYS:HE3	1.84	0.59
1:C:33:ASN:ND2	1:C:58:THR:O	2.36	0.59
1:A:137:LEU:HD23	1:A:138:MET:N	2.18	0.59
1:C:300:ILE:HD11	1:C:301:PHE:CE1	2.37	0.59
1:E:185:LEU:HD11	1:E:261:ILE:HG23	1.83	0.59
1:C:67:ILE:CG2	1:C:91:LEU:HD23	2.33	0.58
1:B:47:VAL:CG2	1:B:72:VAL:HG13	2.33	0.58
1:C:67:ILE:HG22	1:C:67:ILE:O	2.04	0.58
1:A:64:ILE:HD12	1:A:139:PHE:CE1	2.38	0.58
1:D:33:ASN:ND2	1:D:58:THR:O	2.36	0.58
1:D:67:ILE:HD11	1:D:139:PHE:O	2.03	0.58
1:E:221:LEU:CD1	1:E:225:ILE:HD11	2.32	0.58
1:A:108:ILE:CD1	1:A:235:LEU:HD21	2.33	0.58
1:B:99:VAL:HG23	1:B:108:ILE:HG12	1.84	0.58
1:C:275:LEU:O	1:C:276:LEU:C	2.45	0.58
1:B:302:MET:CE	1:C:298:ALA:HA	2.27	0.57
1:D:333:VAL:HA	1:D:336:VAL:HG12	1.86	0.57
1:C:122:LEU:HD22	1:C:217:ASN:ND2	2.19	0.57
1:A:302:MET:HE3	1:B:301:PHE:HB2	1.85	0.57
1:B:225:ILE:HG21	1:B:261:ILE:HG22	1.85	0.57
1:E:199:VAL:HG13	1:E:279:TYR:HA	1.86	0.57
1:A:177:LEU:HD23	1:A:181:TYR:HE2	1.69	0.57
1:C:296:ILE:HA	1:C:299:THR:HG22	1.85	0.57
1:C:333:VAL:HA	1:C:336:VAL:HG12	1.85	0.57
1:C:185:LEU:HD13	1:C:264:THR:HG21	1.86	0.57
1:E:202:ARG:N	1:E:203:PRO:HD3	2.19	0.57
1:E:113:PHE:HB2	1:E:184:LEU:HD21	1.85	0.57
1:D:285:ASN:O	1:D:288:ASN:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:THR:CG2	1:E:276:LEU:HD13	2.34	0.57
1:A:225:ILE:N	1:A:225:ILE:HD12	2.20	0.57
1:D:240:PRO:HB2	1:D:241:PRO:HD3	1.87	0.57
1:A:327:TYR:HA	1:E:315:PHE:CZ	2.40	0.57
1:B:33:ASN:CG	1:B:60:THR:HG22	2.30	0.57
1:D:225:ILE:O	1:D:229:ARG:N	2.37	0.56
1:A:296:ILE:HD12	1:A:297:ILE:N	2.20	0.56
1:B:48:GLU:HA	1:B:51:LEU:HD13	1.88	0.56
1:D:299:THR:HG21	1:D:345:PHE:CZ	2.40	0.56
1:A:31:VAL:HA	1:A:61:TRP:O	2.05	0.56
1:A:268:PHE:C	1:A:270:ASP:H	2.13	0.56
1:B:296:ILE:HD11	1:B:297:ILE:CD1	2.35	0.56
1:C:171:TYR:CD1	1:C:251:PHE:HB3	2.39	0.56
1:C:296:ILE:HD11	1:C:297:ILE:HD12	1.87	0.56
1:C:296:ILE:HD12	1:C:297:ILE:HD12	1.86	0.56
1:D:268:PHE:C	1:D:270:ASP:H	2.13	0.56
1:B:147:PHE:O	1:B:150:VAL:HG12	2.05	0.56
1:D:26:ASP:O	1:D:68:HIS:NE2	2.32	0.56
1:E:44:THR:HG21	1:E:49:SER:OG	2.06	0.56
1:A:290:VAL:HG13	1:E:295:THR:OG1	2.05	0.56
1:A:219:VAL:HG22	1:A:269:ARG:HE	1.69	0.56
1:B:310:ILE:HG22	1:B:311:TYR:CD1	2.40	0.56
1:C:122:LEU:CD2	1:C:217:ASN:ND2	2.69	0.56
1:C:300:ILE:HG13	1:C:301:PHE:N	2.21	0.56
1:D:112:MET:HE1	1:D:146:VAL:N	2.21	0.56
1:B:73:VAL:CG1	1:B:87:LEU:HD22	2.36	0.56
1:C:71:ASP:OD1	1:C:72:VAL:N	2.39	0.56
1:B:138:MET:HE3	1:B:140:GLN:HE21	1.71	0.56
1:C:239:VAL:HB	1:C:242:LEU:HD23	1.87	0.56
1:E:27:PHE:CZ	1:E:72:VAL:HG21	2.41	0.56
1:B:171:TYR:OH	1:B:235:LEU:HG	2.05	0.56
1:E:225:ILE:HG22	1:E:262:ALA:HB2	1.88	0.56
1:C:99:VAL:HB	1:C:231:VAL:HG13	1.88	0.55
1:D:235:LEU:O	1:D:239:VAL:HG22	2.06	0.55
1:B:190:ASP:O	1:B:194:VAL:HG23	2.06	0.55
1:D:196:GLU:O	1:D:200:LEU:HD22	2.05	0.55
1:C:70:THR:HG22	1:C:91:LEU:CD2	2.32	0.55
1:A:311:TYR:HB2	1:E:313:MET:SD	2.47	0.55
1:E:270:ASP:O	1:E:273:SER:OG	2.24	0.55
1:C:232:LEU:HD23	1:C:255:TYR:N	2.22	0.55
1:A:331:LEU:HD12	1:A:334:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:ASN:CG	1:E:60:THR:HG22	2.32	0.55
1:E:63:ASN:HB2	1:E:138:MET:HE2	1.88	0.55
1:E:213:GLN:O	1:E:216:ARG:HB3	2.07	0.55
1:A:151:ARG:O	1:A:154:ILE:HB	2.06	0.55
1:A:170:LEU:O	1:A:172:SER:N	2.34	0.55
1:B:240:PRO:HB2	1:B:241:PRO:HD3	1.88	0.55
1:D:53:PHE:O	1:D:54:ARG:C	2.50	0.55
1:E:150:VAL:HG11	1:E:173:LEU:CD2	2.36	0.55
1:E:221:LEU:HG	1:E:225:ILE:CD1	2.25	0.55
1:E:226:TRP:N	1:E:227:PRO:HD2	2.21	0.55
1:A:112:MET:HE1	1:A:146:VAL:HG13	1.88	0.55
1:C:218:LEU:HD21	1:C:268:PHE:HB3	1.88	0.55
1:A:251:PHE:HA	1:A:254:VAL:HG23	1.88	0.54
1:B:149:PRO:O	1:B:153:ARG:HG3	2.06	0.54
1:C:51:LEU:N	1:C:52:PRO:HD2	2.23	0.54
1:C:171:TYR:O	1:C:250:TYR:CE2	2.59	0.54
1:C:295:THR:O	1:C:299:THR:HG22	2.06	0.54
1:E:254:VAL:O	1:E:255:TYR:C	2.50	0.54
1:B:171:TYR:CD1	1:B:251:PHE:HB3	2.42	0.54
1:C:167:ASP:OD1	1:C:168:TYR:N	2.40	0.54
1:B:238:ASP:C	1:B:239:VAL:HG23	2.32	0.54
1:B:294:LEU:HD23	1:B:294:LEU:O	2.07	0.54
1:C:174:ILE:HD13	1:C:232:LEU:HD11	1.90	0.54
1:C:291:MET:CE	1:D:290:VAL:HG12	2.38	0.54
1:A:171:TYR:CD1	1:A:247:THR:HG22	2.43	0.54
1:A:232:LEU:HD23	1:A:255:TYR:N	2.22	0.54
1:A:295:THR:OG1	1:B:290:VAL:HG13	2.07	0.54
1:D:202:ARG:N	1:D:203:PRO:HD3	2.22	0.54
1:D:238:ASP:C	1:D:239:VAL:HG23	2.31	0.54
1:D:293:VAL:O	1:D:294:LEU:C	2.51	0.54
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.90	0.54
1:A:221:LEU:O	1:A:225:ILE:HD12	2.07	0.54
1:D:51:LEU:N	1:D:52:PRO:HD2	2.23	0.54
1:D:132:THR:HG23	1:D:135:CYS:HB2	1.90	0.54
1:D:232:LEU:HD23	1:D:255:TYR:N	2.23	0.54
1:D:85:LEU:H	1:D:85:LEU:HD23	1.73	0.54
1:D:90:ILE:HG23	1:D:128:SER:OG	2.08	0.54
1:A:292:LYS:O	1:A:296:ILE:HG23	2.08	0.54
1:B:85:LEU:HD23	1:B:85:LEU:H	1.73	0.54
1:D:99:VAL:HG11	1:D:234:SER:HB3	1.89	0.54
1:E:330:VAL:CG1	1:E:331:LEU:HD12	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:MET:HE2	1:C:290:VAL:HG12	1.88	0.53
1:A:67:ILE:HG13	1:A:140:GLN:O	2.09	0.53
1:B:291:MET:CE	1:C:290:VAL:CG1	2.84	0.53
1:A:152:GLU:OE1	1:A:156:TYR:CD2	2.61	0.53
1:A:291:MET:HE3	1:B:290:VAL:HG12	1.89	0.53
1:C:202:ARG:N	1:C:203:PRO:HD3	2.23	0.53
1:E:51:LEU:N	1:E:52:PRO:HD2	2.24	0.53
1:A:130:ILE:HD12	1:A:139:PHE:CE2	2.43	0.53
1:A:152:GLU:OE1	1:A:156:TYR:CE2	2.62	0.53
1:A:296:ILE:O	1:A:299:THR:HG22	2.07	0.53
1:B:51:LEU:N	1:B:52:PRO:HD2	2.24	0.53
1:B:294:LEU:C	1:B:294:LEU:CD2	2.77	0.53
1:C:294:LEU:C	1:C:294:LEU:HD23	2.32	0.53
1:D:232:LEU:HD21	1:D:254:VAL:HG12	1.90	0.53
1:D:291:MET:O	1:D:295:THR:OG1	2.26	0.53
1:D:300:ILE:HG22	1:D:341:MET:HG2	1.90	0.53
1:E:293:VAL:HG12	1:E:294:LEU:N	2.24	0.53
1:A:330:VAL:O	1:A:333:VAL:HG12	2.08	0.53
1:D:150:VAL:HG11	1:D:173:LEU:HD23	1.89	0.53
1:E:165:ARG:HD3	1:E:243:ILE:HD11	1.90	0.53
1:E:256:ASP:O	1:E:257:HIS:C	2.52	0.53
1:A:185:LEU:O	1:A:186:GLU:C	2.51	0.53
1:C:117:LYS:O	1:C:118:ASN:HB2	2.09	0.53
1:D:315:PHE:CE2	1:E:327:TYR:HA	2.44	0.53
1:E:171:TYR:OH	1:E:235:LEU:HG	2.08	0.53
1:E:199:VAL:HG12	1:E:278:VAL:HG12	1.90	0.53
1:B:327:TYR:HB3	1:B:328:PRO:HD3	1.91	0.53
1:D:235:LEU:O	1:D:239:VAL:CG2	2.57	0.53
1:D:304:LEU:HD11	1:D:338:ALA:HB2	1.90	0.53
1:A:85:LEU:H	1:A:85:LEU:HD23	1.74	0.53
1:B:150:VAL:HG11	1:B:173:LEU:HD23	1.90	0.53
1:E:236:TYR:HA	1:E:251:PHE:CZ	2.37	0.53
1:B:313:MET:HE1	1:C:308:ALA:O	2.10	0.52
1:C:192:ILE:O	1:C:193:ASP:C	2.51	0.52
1:D:313:MET:HE2	1:D:313:MET:HA	1.89	0.52
1:E:33:ASN:HA	1:E:60:THR:HA	1.91	0.52
1:A:61:TRP:HB2	1:A:169:LEU:HD21	1.92	0.52
1:E:264:THR:O	1:E:265:VAL:C	2.52	0.52
1:B:277:ASP:HB3	1:C:276:LEU:HD23	1.91	0.52
1:C:31:VAL:HG22	1:C:62:ILE:HG23	1.91	0.52
1:B:27:PHE:CZ	1:B:29:ILE:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LEU:HD22	1:D:139:PHE:CZ	2.45	0.52
1:D:171:TYR:CD1	1:D:247:THR:HG22	2.45	0.52
1:D:295:THR:HA	1:E:294:LEU:HD12	1.91	0.52
1:B:31:VAL:HG21	1:B:50:VAL:CG1	2.39	0.52
1:B:109:VAL:O	1:B:110:LEU:HD23	2.10	0.52
1:C:33:ASN:ND2	1:C:60:THR:HG22	2.23	0.52
1:B:136:VAL:CG2	1:B:169:LEU:HD23	2.40	0.52
1:C:181:TYR:CB	1:C:261:ILE:HD13	2.40	0.52
1:A:145:ASP:OD1	1:A:147:PHE:N	2.39	0.51
1:C:303:PRO:HA	1:C:306:PHE:HB3	1.91	0.51
1:A:156:TYR:O	1:A:157:ASN:C	2.53	0.51
1:E:156:TYR:O	1:E:157:ASN:C	2.54	0.51
1:B:296:ILE:HD11	1:B:297:ILE:HD12	1.91	0.51
1:D:224:THR:O	1:D:224:THR:CG2	2.57	0.51
1:A:286:LYS:O	1:A:287:THR:C	2.53	0.51
1:A:290:VAL:CG1	1:E:291:MET:HE3	2.41	0.51
1:E:33:ASN:ND2	1:E:60:THR:HG22	2.24	0.51
1:A:136:VAL:HG11	1:A:173:LEU:HD12	1.93	0.51
1:B:132:THR:HG23	1:B:132:THR:O	2.11	0.51
1:B:295:THR:O	1:B:299:THR:HB	2.09	0.51
1:C:154:ILE:CG1	1:C:161:ILE:HG21	2.40	0.51
1:D:82:ILE:HD13	1:D:130:ILE:HD13	1.92	0.51
1:B:225:ILE:HG21	1:B:261:ILE:CG2	2.41	0.51
1:B:330:VAL:O	1:B:333:VAL:HG12	2.11	0.51
1:A:112:MET:CE	1:A:146:VAL:HG22	2.41	0.51
1:B:165:ARG:HD3	1:B:243:ILE:HD11	1.93	0.51
1:A:67:ILE:O	1:A:67:ILE:CG2	2.59	0.51
1:A:112:MET:HE1	1:A:146:VAL:N	2.26	0.51
1:D:302:MET:HE3	1:E:298:ALA:HA	1.93	0.51
1:B:267:THR:O	1:B:271:ILE:HD12	2.09	0.51
1:B:291:MET:HE3	1:C:290:VAL:CG1	2.41	0.51
1:B:313:MET:N	1:B:313:MET:HE2	2.25	0.51
1:C:166:ALA:O	1:C:169:LEU:HB3	2.11	0.51
1:D:330:VAL:HG13	1:D:334:MET:HE2	1.93	0.51
1:A:48:GLU:HA	1:A:51:LEU:HD13	1.92	0.50
1:B:99:VAL:HB	1:B:231:VAL:HG13	1.93	0.50
1:C:240:PRO:HB2	1:C:241:PRO:HD3	1.92	0.50
1:D:47:VAL:O	1:D:50:VAL:HG22	2.11	0.50
1:D:296:ILE:HG22	1:D:345:PHE:CE2	2.46	0.50
1:E:67:ILE:HD11	1:E:139:PHE:O	2.11	0.50
1:A:291:MET:HE2	1:B:291:MET:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:C	1:D:172:SER:H	2.19	0.50
1:D:296:ILE:HA	1:D:299:THR:HG22	1.93	0.50
1:E:267:THR:HG22	1:E:271:ILE:CD1	2.41	0.50
1:E:330:VAL:HG13	1:E:331:LEU:N	2.25	0.50
1:A:132:THR:HG23	1:A:135:CYS:HB2	1.93	0.50
1:B:219:VAL:HG22	1:B:269:ARG:HE	1.76	0.50
1:C:184:LEU:O	1:C:185:LEU:C	2.54	0.50
1:D:236:TYR:OH	1:D:252:ARG:HD2	2.11	0.50
1:D:289:GLU:O	1:D:290:VAL:C	2.55	0.50
1:A:73:VAL:CG1	1:A:87:LEU:HD22	2.40	0.50
1:C:188:ILE:O	1:C:189:ASP:C	2.52	0.50
1:C:199:VAL:HG11	1:C:278:VAL:HB	1.93	0.50
1:E:212:HIS:O	1:E:213:GLN:C	2.54	0.50
1:A:327:TYR:O	1:A:330:VAL:HG12	2.12	0.50
1:B:221:LEU:O	1:B:225:ILE:HD12	2.11	0.50
1:C:222:ALA:HB2	1:C:265:VAL:CG1	2.42	0.50
1:E:200:LEU:HD13	1:E:200:LEU:H	1.76	0.50
1:E:204:GLU:O	1:E:279:TYR:OH	2.27	0.50
1:A:186:GLU:O	1:A:187:LYS:C	2.53	0.50
1:D:243:ILE:HG22	1:D:246:GLU:HB2	1.94	0.50
1:D:291:MET:HE1	1:E:291:MET:HA	1.93	0.50
1:D:313:MET:HE1	1:E:308:ALA:O	2.11	0.50
1:E:61:TRP:HB2	1:E:169:LEU:HD21	1.92	0.50
1:A:243:ILE:HG22	1:A:246:GLU:HB2	1.93	0.50
1:B:250:TYR:C	1:B:250:TYR:CD2	2.90	0.50
1:D:67:ILE:HG13	1:D:140:GLN:O	2.12	0.50
1:D:156:TYR:O	1:D:157:ASN:C	2.54	0.50
1:C:132:THR:HG23	1:C:135:CYS:HB2	1.94	0.49
1:D:225:ILE:HD13	1:D:265:VAL:HG21	1.94	0.49
1:E:47:VAL:O	1:E:50:VAL:HG22	2.12	0.49
1:D:298:ALA:O	1:D:302:MET:CG	2.61	0.49
1:E:195:LEU:HD11	1:E:210:ARG:HD3	1.93	0.49
1:E:199:VAL:CG1	1:E:278:VAL:HG12	2.42	0.49
1:A:67:ILE:HD11	1:A:139:PHE:O	2.13	0.49
1:D:48:GLU:OE1	1:D:51:LEU:HD22	2.13	0.49
1:E:256:ASP:O	1:E:259:ILE:N	2.43	0.49
1:B:26:ASP:O	1:B:68:HIS:NE2	2.40	0.49
1:A:33:ASN:HB2	1:A:60:THR:HG22	1.95	0.49
1:C:82:ILE:HD13	1:C:130:ILE:HD13	1.95	0.49
1:A:259:ILE:HG22	1:A:260:GLN:N	2.28	0.49
1:E:333:VAL:O	1:E:336:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:CG2	1:B:91:LEU:HD23	2.42	0.49
1:A:26:ASP:O	1:A:68:HIS:NE2	2.45	0.49
1:B:136:VAL:HG21	1:B:169:LEU:HB3	1.95	0.49
1:B:221:LEU:CG	1:B:225:ILE:HD11	2.18	0.49
1:A:33:ASN:CB	1:A:60:THR:HG22	2.43	0.49
1:A:221:LEU:HD11	1:A:225:ILE:HD11	1.90	0.49
1:B:298:ALA:O	1:B:302:MET:HG2	2.13	0.49
1:C:171:TYR:CE1	1:C:251:PHE:CD2	3.00	0.49
1:D:88:GLU:HA	1:D:91:LEU:HD12	1.93	0.49
1:E:131:LEU:HD12	1:E:132:THR:N	2.27	0.49
1:A:294:LEU:HD11	1:E:294:LEU:CD2	2.43	0.48
1:D:309:GLY:O	1:D:313:MET:HE3	2.12	0.48
1:E:31:VAL:HA	1:E:61:TRP:O	2.13	0.48
1:E:232:LEU:HD23	1:E:255:TYR:N	2.28	0.48
1:A:264:THR:O	1:A:267:THR:N	2.45	0.48
1:B:93:VAL:HG11	1:B:141:GLU:OE1	2.13	0.48
1:D:197:GLU:HA	1:D:200:LEU:HD23	1.95	0.48
1:E:131:LEU:HD12	1:E:132:THR:H	1.77	0.48
1:B:129:LEU:HD13	1:B:170:LEU:CD1	2.44	0.48
1:C:174:ILE:HG22	1:C:254:VAL:HG11	1.95	0.48
1:D:119:LEU:HD12	1:D:119:LEU:C	2.39	0.48
1:E:232:LEU:HD21	1:E:254:VAL:HG12	1.95	0.48
1:A:235:LEU:O	1:A:239:VAL:HG22	2.14	0.48
1:B:156:TYR:O	1:B:157:ASN:C	2.56	0.48
1:B:296:ILE:CD1	1:B:297:ILE:CD1	2.91	0.48
1:E:272:VAL:O	1:E:273:SER:C	2.57	0.48
1:A:171:TYR:CD1	1:A:251:PHE:HB3	2.48	0.48
1:C:214:LEU:O	1:C:215:LYS:C	2.55	0.48
1:C:226:TRP:N	1:C:227:PRO:HD2	2.28	0.48
1:E:239:VAL:HB	1:E:242:LEU:HD23	1.96	0.48
1:C:188:ILE:HG22	1:C:268:PHE:CE2	2.49	0.48
1:C:219:VAL:HG22	1:C:269:ARG:HE	1.79	0.48
1:C:295:THR:CG2	1:D:293:VAL:HG12	2.43	0.48
1:D:33:ASN:HA	1:D:60:THR:HA	1.94	0.48
1:D:295:THR:HG23	1:E:294:LEU:CB	2.40	0.48
1:E:67:ILE:O	1:E:67:ILE:CG2	2.61	0.48
1:C:82:ILE:HD13	1:C:130:ILE:CD1	2.44	0.48
1:D:202:ARG:O	1:D:204:GLU:N	2.47	0.48
1:E:296:ILE:CG2	1:E:345:PHE:CE2	2.93	0.48
1:A:202:ARG:N	1:A:203:PRO:HD3	2.28	0.48
1:A:296:ILE:HA	1:A:345:PHE:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:HD11	1:B:139:PHE:O	2.14	0.48
1:D:315:PHE:CZ	1:E:327:TYR:HA	2.49	0.48
1:D:48:GLU:O	1:D:50:VAL:N	2.47	0.47
1:C:181:TYR:HB3	1:C:261:ILE:HD13	1.96	0.47
1:E:292:LYS:HD3	1:E:348:LYS:HG2	1.96	0.47
1:A:51:LEU:N	1:A:52:PRO:HD2	2.30	0.47
1:A:137:LEU:HD23	1:A:138:MET:H	1.80	0.47
1:A:196:GLU:HG2	1:A:200:LEU:HD21	1.95	0.47
1:C:302:MET:HB2	1:C:303:PRO:CD	2.44	0.47
1:C:309:GLY:O	1:C:313:MET:HE3	2.14	0.47
1:E:232:LEU:HD21	1:E:254:VAL:CG1	2.45	0.47
1:A:137:LEU:HD22	1:A:139:PHE:CZ	2.50	0.47
1:B:306:PHE:CE1	1:C:304:LEU:HB3	2.50	0.47
1:A:348:LYS:HZ2	1:B:290:VAL:HG22	1.80	0.47
1:C:148:ASP:N	1:C:149:PRO:HD2	2.30	0.47
1:D:33:ASN:HD22	1:D:34:TYR:N	2.13	0.47
1:D:211:THR:O	1:D:211:THR:HG22	2.15	0.47
1:E:224:THR:O	1:E:224:THR:HG22	2.15	0.47
1:A:33:ASN:ND2	1:A:60:THR:HG22	2.30	0.47
1:A:153:ARG:NE	1:A:161:ILE:HD11	2.29	0.47
1:A:195:LEU:HG	1:A:210:ARG:HD3	1.97	0.47
1:C:171:TYR:CD1	1:C:247:THR:HG22	2.50	0.47
1:C:243:ILE:O	1:C:244:GLU:C	2.58	0.47
1:C:250:TYR:C	1:C:250:TYR:CD2	2.93	0.47
1:E:333:VAL:HA	1:E:336:VAL:HG12	1.95	0.47
1:B:131:LEU:HD21	1:B:167:ASP:CB	2.45	0.47
1:B:296:ILE:CA	1:B:299:THR:HG22	2.45	0.47
1:C:221:LEU:O	1:C:225:ILE:HD12	2.14	0.47
1:A:109:VAL:O	1:A:110:LEU:HD23	2.15	0.47
1:A:136:VAL:HG11	1:A:173:LEU:CD1	2.44	0.47
1:A:311:TYR:N	1:A:311:TYR:CD1	2.83	0.47
1:B:178:VAL:HG13	1:B:261:ILE:CD1	2.45	0.47
1:C:131:LEU:HD21	1:C:167:ASP:HA	1.95	0.47
1:E:85:LEU:HD23	1:E:85:LEU:H	1.79	0.47
1:A:339:VAL:HA	1:A:342:VAL:HG12	1.97	0.47
1:B:64:ILE:HD12	1:B:139:PHE:CE1	2.50	0.47
1:B:160:ILE:HG22	1:B:160:ILE:O	2.15	0.47
1:B:286:LYS:O	1:B:287:THR:C	2.58	0.47
1:B:298:ALA:O	1:B:302:MET:CG	2.63	0.47
1:C:33:ASN:HA	1:C:60:THR:HA	1.96	0.47
1:D:171:TYR:HB3	1:D:250:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:VAL:CG1	1:D:294:LEU:N	2.78	0.47
1:B:296:ILE:HA	1:B:299:THR:CG2	2.45	0.46
1:D:169:LEU:O	1:D:170:LEU:C	2.58	0.46
1:D:270:ASP:OD2	1:E:269:ARG:NH1	2.48	0.46
1:D:336:VAL:HG13	1:D:337:ILE:N	2.30	0.46
1:E:138:MET:HE3	1:E:140:GLN:HE21	1.79	0.46
1:E:197:GLU:CA	1:E:200:LEU:HD22	2.40	0.46
1:A:32:MET:HE2	1:A:154:ILE:HG21	1.97	0.46
1:A:63:ASN:HB2	1:A:138:MET:HE2	1.97	0.46
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.73	0.46
1:A:226:TRP:N	1:A:227:PRO:HD2	2.31	0.46
1:B:153:ARG:NE	1:B:161:ILE:HD11	2.30	0.46
1:B:171:TYR:O	1:B:250:TYR:CE2	2.68	0.46
1:C:306:PHE:CE1	1:D:304:LEU:HB3	2.49	0.46
1:D:67:ILE:O	1:D:67:ILE:CG2	2.60	0.46
1:A:313:MET:HE2	1:A:313:MET:HA	1.98	0.46
1:A:327:TYR:HA	1:E:315:PHE:CE2	2.51	0.46
1:C:122:LEU:HD23	1:C:122:LEU:H	1.79	0.46
1:C:333:VAL:O	1:C:336:VAL:HG12	2.16	0.46
1:D:215:LYS:O	1:D:216:ARG:C	2.57	0.46
1:D:313:MET:HE2	1:D:313:MET:CA	2.44	0.46
1:A:110:LEU:HD22	1:A:228:LEU:CD1	2.45	0.46
1:A:224:THR:O	1:A:224:THR:CG2	2.63	0.46
1:A:286:LYS:O	1:A:289:GLU:N	2.49	0.46
1:B:67:ILE:O	1:B:67:ILE:CG2	2.62	0.46
1:C:29:ILE:HG23	1:C:63:ASN:O	2.15	0.46
1:C:156:TYR:O	1:C:157:ASN:C	2.58	0.46
1:C:222:ALA:HB2	1:C:265:VAL:HG11	1.96	0.46
1:C:296:ILE:O	1:C:299:THR:HG22	2.16	0.46
1:D:48:GLU:C	1:D:50:VAL:H	2.24	0.46
1:E:255:TYR:O	1:E:256:ASP:C	2.57	0.46
1:A:331:LEU:HA	1:A:334:MET:HE3	1.98	0.46
1:B:296:ILE:C	1:B:299:THR:HG22	2.41	0.46
1:C:122:LEU:CD2	1:C:217:ASN:HD22	2.28	0.46
1:C:137:LEU:HD22	1:C:139:PHE:CZ	2.50	0.46
1:D:330:VAL:CG1	1:D:331:LEU:HD12	2.44	0.46
1:E:171:TYR:CE1	1:E:251:PHE:CG	3.04	0.46
1:E:283:VAL:O	1:E:286:LYS:N	2.48	0.46
1:E:309:GLY:O	1:E:313:MET:HE3	2.14	0.46
1:A:184:LEU:O	1:A:185:LEU:C	2.59	0.46
1:A:294:LEU:HD11	1:E:294:LEU:HD22	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ILE:HD12	1:A:296:ILE:C	2.40	0.46
1:B:293:VAL:O	1:B:296:ILE:HG13	2.15	0.46
1:E:171:TYR:CE1	1:E:251:PHE:CD2	3.03	0.46
1:E:192:ILE:HG22	1:E:193:ASP:N	2.30	0.46
1:A:240:PRO:CB	1:A:241:PRO:HD3	2.46	0.46
1:B:82:ILE:HG22	1:B:83:HIS:O	2.16	0.46
1:C:333:VAL:C	1:C:336:VAL:HG12	2.41	0.46
1:A:33:ASN:HA	1:A:60:THR:HA	1.96	0.46
1:B:117:LYS:O	1:B:118:ASN:HB2	2.16	0.46
1:C:174:ILE:O	1:C:175:ASP:C	2.57	0.46
1:D:171:TYR:O	1:D:250:TYR:CZ	2.69	0.46
1:D:232:LEU:HD21	1:D:254:VAL:CG1	2.44	0.46
1:A:86:VAL:HG13	1:A:107:PHE:CD2	2.51	0.46
1:A:202:ARG:O	1:A:204:GLU:N	2.49	0.46
1:A:221:LEU:CG	1:A:225:ILE:HD11	2.45	0.46
1:B:146:VAL:HG11	1:B:180:ASP:HB2	1.97	0.46
1:D:195:LEU:HD11	1:D:210:ARG:HD3	1.98	0.46
1:B:296:ILE:HD12	1:B:297:ILE:N	2.31	0.45
1:D:151:ARG:O	1:D:154:ILE:HB	2.15	0.45
1:E:279:TYR:O	1:E:280:LEU:C	2.59	0.45
1:A:136:VAL:CG2	1:A:169:LEU:HD23	2.47	0.45
1:B:202:ARG:O	1:B:204:GLU:N	2.50	0.45
1:C:225:ILE:CG2	1:C:262:ALA:HB2	2.45	0.45
1:D:183:VAL:O	1:D:184:LEU:C	2.58	0.45
1:B:199:VAL:HG13	1:B:279:TYR:HA	1.98	0.45
1:B:291:MET:HE3	1:B:291:MET:O	2.16	0.45
1:B:306:PHE:CE2	1:B:310:ILE:HD11	2.52	0.45
1:E:199:VAL:HG13	1:E:279:TYR:CA	2.47	0.45
1:C:219:VAL:O	1:C:220:GLU:C	2.59	0.45
1:C:238:ASP:C	1:C:239:VAL:CG2	2.87	0.45
1:D:116:ASP:CG	1:D:119:LEU:HB3	2.41	0.45
1:E:300:ILE:HG22	1:E:341:MET:CG	2.45	0.45
1:B:33:ASN:CB	1:B:60:THR:HG22	2.46	0.45
1:B:313:MET:HE2	1:B:313:MET:CA	2.46	0.45
1:D:180:ASP:O	1:D:183:VAL:HB	2.16	0.45
1:E:200:LEU:HD13	1:E:200:LEU:N	2.32	0.45
1:D:194:VAL:C	1:D:196:GLU:H	2.24	0.45
1:D:224:THR:O	1:D:224:THR:HG22	2.16	0.45
1:E:170:LEU:C	1:E:172:SER:H	2.24	0.45
1:B:148:ASP:N	1:B:149:PRO:HD2	2.31	0.45
1:B:313:MET:HE2	1:B:313:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ASN:CB	1:E:138:MET:HE2	2.47	0.45
1:A:173:LEU:O	1:A:176:ALA:HB3	2.16	0.45
1:B:297:ILE:HG22	1:B:298:ALA:N	2.32	0.45
1:B:303:PRO:O	1:B:306:PHE:HB3	2.17	0.45
1:B:99:VAL:HG21	1:B:235:LEU:HD13	1.99	0.45
1:B:303:PRO:HA	1:B:306:PHE:HB3	1.99	0.45
1:C:67:ILE:HD11	1:C:139:PHE:O	2.17	0.45
1:C:145:ASP:OD1	1:C:147:PHE:N	2.46	0.45
1:E:177:LEU:C	1:E:177:LEU:CD2	2.88	0.45
1:A:152:GLU:OE2	1:A:155:ARG:HD2	2.17	0.45
1:B:192:ILE:O	1:B:193:ASP:C	2.60	0.45
1:E:327:TYR:HB3	1:E:328:PRO:HD3	1.99	0.45
1:A:280:LEU:HD23	1:B:280:LEU:HD21	1.99	0.44
1:C:138:MET:HE3	1:C:140:GLN:HE21	1.82	0.44
1:E:97:PRO:HD3	1:E:111:LYS:HE2	2.00	0.44
1:E:111:LYS:HG2	1:E:126:GLN:HG3	2.00	0.44
1:A:97:PRO:HD3	1:A:111:LYS:HE2	1.99	0.44
1:A:221:LEU:HG	1:A:225:ILE:CD1	2.47	0.44
1:B:330:VAL:CA	1:B:333:VAL:HG12	2.47	0.44
1:C:215:LYS:O	1:C:219:VAL:HG23	2.17	0.44
1:C:236:TYR:HA	1:C:251:PHE:CZ	2.43	0.44
1:D:219:VAL:O	1:D:220:GLU:C	2.60	0.44
1:A:259:ILE:O	1:A:260:GLN:C	2.59	0.44
1:A:333:VAL:HA	1:A:336:VAL:HG12	1.98	0.44
1:C:71:ASP:OD1	1:C:72:VAL:HG23	2.17	0.44
1:C:136:VAL:HG21	1:C:169:LEU:HG	2.00	0.44
1:A:218:LEU:HB3	1:A:269:ARG:HG3	1.99	0.44
1:A:242:LEU:HD12	1:A:242:LEU:H	1.82	0.44
1:A:276:LEU:O	1:A:279:TYR:HB3	2.17	0.44
1:C:108:ILE:HG22	1:C:110:LEU:HG	1.99	0.44
1:C:302:MET:HB2	1:C:303:PRO:HD3	1.98	0.44
1:D:206:GLU:HB2	1:D:209:GLN:HG2	1.99	0.44
1:A:171:TYR:CE1	1:A:251:PHE:CD2	3.06	0.44
1:A:268:PHE:C	1:A:270:ASP:N	2.73	0.44
1:E:47:VAL:HG23	1:E:72:VAL:HG13	2.00	0.44
1:A:32:MET:HE1	1:A:151:ARG:O	2.17	0.44
1:A:87:LEU:O	1:A:90:ILE:HB	2.17	0.44
1:E:330:VAL:CG1	1:E:331:LEU:N	2.81	0.44
1:A:112:MET:HE1	1:A:146:VAL:H	1.81	0.44
1:A:260:GLN:O	1:A:261:ILE:C	2.60	0.44
1:B:171:TYR:CD1	1:B:247:THR:HG22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ILE:CA	1:C:299:THR:HG22	2.48	0.44
1:D:306:PHE:CE2	1:D:310:ILE:HD11	2.53	0.44
1:A:265:VAL:O	1:A:268:PHE:N	2.51	0.44
1:B:209:GLN:HG3	1:B:210:ARG:N	2.32	0.44
1:C:69:ARG:HB3	1:C:72:VAL:HG23	2.00	0.44
1:C:268:PHE:C	1:C:270:ASP:H	2.24	0.44
1:D:171:TYR:CE1	1:D:251:PHE:CD2	3.06	0.44
1:A:167:ASP:OD1	1:A:168:TYR:N	2.51	0.44
1:D:150:VAL:CG1	1:D:151:ARG:N	2.81	0.44
1:E:196:GLU:O	1:E:200:LEU:HD13	2.18	0.44
1:A:296:ILE:HG22	1:A:345:PHE:CE2	2.52	0.43
1:D:125:GLU:OE1	1:D:142:LYS:HG2	2.18	0.43
1:D:313:MET:HA	1:E:311:TYR:O	2.18	0.43
1:E:113:PHE:CB	1:E:184:LEU:HD21	2.47	0.43
1:E:192:ILE:O	1:E:193:ASP:C	2.61	0.43
1:B:152:GLU:OE2	1:B:155:ARG:NH1	2.51	0.43
1:D:295:THR:CA	1:E:294:LEU:HD12	2.47	0.43
1:E:63:ASN:CG	1:E:138:MET:HE2	2.43	0.43
1:E:117:LYS:O	1:E:118:ASN:HB2	2.17	0.43
1:D:177:LEU:C	1:D:177:LEU:CD2	2.88	0.43
1:D:247:THR:O	1:D:250:TYR:HB3	2.17	0.43
1:C:296:ILE:HA	1:C:345:PHE:HE2	1.83	0.43
1:D:90:ILE:HG23	1:D:128:SER:CB	2.49	0.43
1:D:165:ARG:HD3	1:D:243:ILE:HD11	2.01	0.43
1:D:188:ILE:O	1:D:189:ASP:C	2.62	0.43
1:E:214:LEU:HD12	1:E:214:LEU:HA	1.73	0.43
1:E:251:PHE:O	1:E:252:ARG:C	2.61	0.43
1:D:268:PHE:C	1:D:270:ASP:N	2.76	0.43
1:E:286:LYS:O	1:E:287:THR:C	2.60	0.43
1:A:82:ILE:HG22	1:A:83:HIS:O	2.17	0.43
1:A:130:ILE:HB	1:A:137:LEU:HB3	2.01	0.43
1:A:153:ARG:NH2	1:A:161:ILE:HD11	2.33	0.43
1:A:295:THR:OG1	1:B:290:VAL:CG1	2.67	0.43
1:A:305:THR:O	1:A:305:THR:HG22	2.18	0.43
1:B:260:GLN:O	1:B:261:ILE:C	2.61	0.43
1:D:152:GLU:OE1	1:D:156:TYR:CE2	2.70	0.43
1:E:108:ILE:HG22	1:E:110:LEU:HG	2.00	0.43
1:B:339:VAL:O	1:B:342:VAL:HG12	2.18	0.43
1:C:82:ILE:CD1	1:C:130:ILE:HD13	2.49	0.43
1:D:327:TYR:HB3	1:D:328:PRO:HD3	2.00	0.43
1:A:243:ILE:O	1:A:244:GLU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:PHE:C	1:B:270:ASP:H	2.27	0.43
1:D:82:ILE:CD1	1:D:130:ILE:HD13	2.49	0.43
1:D:99:VAL:HG13	1:D:99:VAL:O	2.18	0.43
1:D:296:ILE:HD12	1:D:296:ILE:C	2.44	0.43
1:A:108:ILE:HD11	1:A:235:LEU:CD2	2.43	0.43
1:A:208:VAL:CG2	1:A:279:TYR:CZ	3.01	0.43
1:C:275:LEU:O	1:C:278:VAL:N	2.49	0.43
1:C:327:TYR:HB3	1:C:328:PRO:HD3	2.00	0.43
1:D:112:MET:HE1	1:D:146:VAL:HG13	1.99	0.43
1:D:236:TYR:HA	1:D:251:PHE:CZ	2.39	0.43
1:E:92:ASN:OD1	1:E:92:ASN:C	2.60	0.43
1:E:221:LEU:C	1:E:225:ILE:HD12	2.43	0.43
1:E:225:ILE:CG2	1:E:262:ALA:HB2	2.48	0.43
1:E:228:LEU:HD23	1:E:228:LEU:O	2.19	0.43
1:E:313:MET:N	1:E:313:MET:HE2	2.33	0.43
1:B:82:ILE:HD13	1:B:130:ILE:HD13	2.01	0.42
1:E:313:MET:HE2	1:E:313:MET:HA	2.01	0.42
1:B:289:GLU:O	1:B:290:VAL:C	2.62	0.42
1:B:296:ILE:HG22	1:B:345:PHE:CE2	2.54	0.42
1:C:61:TRP:HB2	1:C:169:LEU:HD21	2.01	0.42
1:D:83:HIS:HB2	1:D:86:VAL:CG2	2.49	0.42
1:D:341:MET:O	1:D:344:TYR:N	2.52	0.42
1:A:47:VAL:HG13	1:A:48:GLU:N	2.35	0.42
1:A:256:ASP:HA	1:A:259:ILE:HD12	2.02	0.42
1:B:153:ARG:HE	1:B:161:ILE:HD11	1.83	0.42
1:E:198:GLU:HA	1:E:202:ARG:HB3	2.01	0.42
1:D:233:SER:HA	1:D:255:TYR:CE1	2.54	0.42
1:D:330:VAL:CG1	1:D:331:LEU:N	2.82	0.42
1:E:148:ASP:N	1:E:149:PRO:HD2	2.34	0.42
1:E:303:PRO:O	1:E:304:LEU:C	2.62	0.42
1:A:221:LEU:HG	1:A:225:ILE:HD11	2.01	0.42
1:C:111:LYS:O	1:C:181:TYR:OH	2.22	0.42
1:E:265:VAL:O	1:E:266:GLU:C	2.61	0.42
1:E:267:THR:C	1:E:271:ILE:HD12	2.44	0.42
1:A:348:LYS:NZ	1:B:290:VAL:HG22	2.34	0.42
1:B:113:PHE:CZ	1:B:224:THR:HG21	2.55	0.42
1:B:296:ILE:HD12	1:B:296:ILE:C	2.45	0.42
1:D:140:GLN:HE22	1:D:145:ASP:CG	2.28	0.42
1:D:147:PHE:O	1:D:148:ASP:C	2.61	0.42
1:D:226:TRP:N	1:D:227:PRO:HD2	2.35	0.42
1:A:113:PHE:CE1	1:A:124:SER:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASP:O	1:C:273:SER:HB3	2.19	0.42
1:C:333:VAL:HA	1:C:336:VAL:CG1	2.49	0.42
1:A:339:VAL:O	1:A:340:ILE:C	2.62	0.42
1:B:221:LEU:O	1:B:224:THR:N	2.44	0.42
1:B:226:TRP:N	1:B:227:PRO:HD2	2.34	0.42
1:C:165:ARG:HD3	1:C:243:ILE:CD1	2.44	0.42
1:D:199:VAL:HG13	1:D:279:TYR:CA	2.49	0.42
1:A:108:ILE:CD1	1:A:235:LEU:CD2	2.97	0.42
1:A:149:PRO:O	1:A:153:ARG:HG3	2.20	0.42
1:B:224:THR:HG22	1:B:224:THR:O	2.20	0.42
1:C:61:TRP:CD1	1:C:61:TRP:C	2.97	0.42
1:C:225:ILE:HD12	1:C:225:ILE:N	2.35	0.42
1:C:333:VAL:CA	1:C:336:VAL:HG12	2.49	0.42
1:D:148:ASP:N	1:D:149:PRO:HD2	2.33	0.42
1:D:149:PRO:O	1:D:153:ARG:HG3	2.19	0.42
1:D:195:LEU:CD1	1:D:210:ARG:HD3	2.50	0.42
1:D:333:VAL:C	1:D:336:VAL:HG12	2.45	0.42
1:B:234:SER:HA	1:B:237:ARG:HG2	2.02	0.42
1:B:306:PHE:CZ	1:B:310:ILE:HD11	2.55	0.42
1:B:336:VAL:HG13	1:B:337:ILE:N	2.34	0.42
1:C:171:TYR:CE1	1:C:251:PHE:CG	3.08	0.42
1:C:192:ILE:HG22	1:C:193:ASP:N	2.34	0.42
1:C:294:LEU:HD23	1:C:294:LEU:O	2.20	0.42
1:C:299:THR:HA	1:D:297:ILE:HG21	2.02	0.42
1:B:61:TRP:CD1	1:B:61:TRP:C	2.98	0.41
1:C:232:LEU:HD21	1:C:254:VAL:HG12	2.01	0.41
1:D:260:GLN:O	1:D:261:ILE:C	2.63	0.41
1:E:339:VAL:HA	1:E:342:VAL:HG12	2.01	0.41
1:E:84:PRO:O	1:E:87:LEU:HB2	2.20	0.41
1:B:302:MET:HB2	1:B:303:PRO:CD	2.50	0.41
1:D:244:GLU:O	1:D:248:VAL:HB	2.20	0.41
1:D:277:ASP:O	1:D:278:VAL:C	2.62	0.41
1:E:300:ILE:HG22	1:E:341:MET:HG2	2.03	0.41
1:A:152:GLU:HA	1:A:155:ARG:HB2	2.01	0.41
1:B:67:ILE:HG22	1:B:91:LEU:HD23	2.01	0.41
1:B:196:GLU:HG2	1:B:200:LEU:HD21	2.02	0.41
1:C:302:MET:HE2	1:D:301:PHE:HB2	2.02	0.41
1:D:333:VAL:CA	1:D:336:VAL:HG12	2.50	0.41
1:A:108:ILE:HG22	1:A:109:VAL:N	2.35	0.41
1:B:268:PHE:C	1:B:270:ASP:N	2.79	0.41
1:B:303:PRO:C	1:B:306:PHE:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ILE:CG2	1:C:67:ILE:O	2.67	0.41
1:C:170:LEU:C	1:C:172:SER:H	2.27	0.41
1:C:173:LEU:O	1:C:174:ILE:C	2.62	0.41
1:D:330:VAL:HG13	1:D:331:LEU:N	2.35	0.41
1:E:205:LYS:HD3	1:E:205:LYS:C	2.46	0.41
1:C:160:ILE:HG23	1:C:163:LYS:HD2	2.02	0.41
1:E:331:LEU:HA	1:E:334:MET:HE3	2.02	0.41
1:A:339:VAL:O	1:A:341:MET:N	2.54	0.41
1:B:72:VAL:O	1:B:76:VAL:HG23	2.20	0.41
1:B:195:LEU:HD11	1:B:210:ARG:HD3	2.02	0.41
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.87	0.41
1:D:198:GLU:OE2	1:D:210:ARG:NH1	2.54	0.41
1:E:62:ILE:O	1:E:137:LEU:HD23	2.20	0.41
1:E:83:HIS:HB3	1:E:84:PRO:HD2	2.02	0.41
1:A:191:GLU:HG3	1:A:195:LEU:HD22	2.01	0.41
1:A:199:VAL:HG13	1:A:279:TYR:CA	2.49	0.41
1:C:232:LEU:CD2	1:C:254:VAL:HG12	2.50	0.41
1:C:299:THR:HG21	1:C:345:PHE:CE2	2.56	0.41
1:D:313:MET:HE2	1:D:313:MET:N	2.36	0.41
1:A:67:ILE:HD11	1:A:139:PHE:C	2.45	0.41
1:A:221:LEU:O	1:A:225:ILE:CD1	2.67	0.41
1:A:247:THR:O	1:A:250:TYR:HB3	2.21	0.41
1:B:134:ASN:HA	1:B:166:ALA:HB3	2.02	0.41
1:C:67:ILE:HD11	1:C:139:PHE:HB3	2.02	0.41
1:C:99:VAL:HG21	1:C:235:LEU:CD1	2.29	0.41
1:C:116:ASP:O	1:C:119:LEU:O	2.38	0.41
1:C:225:ILE:HG21	1:C:261:ILE:HG22	2.03	0.41
1:E:263:ASP:O	1:E:264:THR:C	2.64	0.41
1:E:296:ILE:O	1:E:299:THR:HG22	2.21	0.41
1:A:153:ARG:HE	1:A:161:ILE:HD11	1.85	0.41
1:B:295:THR:CG2	1:C:293:VAL:HG12	2.50	0.41
1:C:264:THR:O	1:C:267:THR:HB	2.21	0.41
1:C:302:MET:HE1	1:D:302:MET:HG2	2.03	0.41
1:D:113:PHE:CE2	1:D:221:LEU:HD12	2.56	0.41
1:D:137:LEU:HD22	1:D:139:PHE:CE2	2.56	0.41
1:E:109:VAL:HG13	1:E:128:SER:OG	2.21	0.41
1:C:67:ILE:HG13	1:C:140:GLN:O	2.21	0.40
1:D:268:PHE:O	1:D:270:ASP:N	2.54	0.40
1:A:239:VAL:CG1	1:A:242:LEU:HB3	2.51	0.40
1:A:333:VAL:C	1:A:336:VAL:HG12	2.46	0.40
1:B:89:ASP:HB3	1:B:95:GLN:HE22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HB	1:B:242:LEU:HD23	2.03	0.40
1:C:300:ILE:CG1	1:C:301:PHE:N	2.84	0.40
1:D:168:TYR:O	1:D:169:LEU:C	2.61	0.40
1:D:231:VAL:O	1:D:235:LEU:HB2	2.21	0.40
1:E:243:ILE:O	1:E:244:GLU:C	2.64	0.40
1:E:313:MET:HE2	1:E:313:MET:CA	2.51	0.40
1:A:330:VAL:HG13	1:A:331:LEU:N	2.37	0.40
1:B:191:GLU:O	1:B:192:ILE:C	2.64	0.40
1:C:221:LEU:CG	1:C:225:ILE:HD11	2.44	0.40
1:D:109:VAL:O	1:D:110:LEU:HD23	2.21	0.40
1:D:333:VAL:O	1:D:336:VAL:HG12	2.21	0.40
1:E:226:TRP:N	1:E:227:PRO:CD	2.84	0.40
1:E:261:ILE:C	1:E:263:ASP:N	2.80	0.40
1:A:148:ASP:N	1:A:149:PRO:HD2	2.37	0.40
1:A:166:ALA:O	1:A:169:LEU:HB3	2.22	0.40
1:B:228:LEU:C	1:B:228:LEU:HD23	2.46	0.40
1:B:279:TYR:O	1:B:280:LEU:C	2.63	0.40
1:C:27:PHE:CZ	1:C:72:VAL:HG21	2.57	0.40
1:C:184:LEU:O	1:C:187:LYS:N	2.55	0.40
1:D:99:VAL:O	1:D:99:VAL:HG22	2.21	0.40
1:D:168:TYR:CD2	1:D:168:TYR:C	2.99	0.40
1:D:191:GLU:CG	1:D:195:LEU:HD22	2.50	0.40
1:E:122:LEU:HD23	1:E:122:LEU:H	1.86	0.40
1:E:188:ILE:HD13	1:E:188:ILE:HG21	1.88	0.40
1:E:207:THR:O	1:E:208:VAL:C	2.63	0.40
1:A:339:VAL:C	1:A:341:MET:N	2.78	0.40
1:E:171:TYR:CD1	1:E:247:THR:HG22	2.56	0.40
1:E:302:MET:HB2	1:E:303:PRO:CD	2.51	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	310/330 (94%)	258 (83%)	44 (14%)	8 (3%)	4	28
1	B	310/330 (94%)	257 (83%)	44 (14%)	9 (3%)	3	26
1	C	310/330 (94%)	255 (82%)	49 (16%)	6 (2%)	6	33
1	D	310/330 (94%)	250 (81%)	48 (16%)	12 (4%)	2	22
1	E	310/330 (94%)	258 (83%)	47 (15%)	5 (2%)	7	36
All	All	1550/1650 (94%)	1278 (82%)	232 (15%)	40 (3%)	4	28

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	244	GLU
1	B	244	GLU
1	C	157	ASN
1	A	157	ASN
1	A	240	PRO
1	B	157	ASN
1	C	244	GLU
1	D	119	LEU
1	D	157	ASN
1	E	157	ASN
1	E	244	GLU
1	B	240	PRO
1	D	49	SER
1	D	240	PRO
1	D	244	GLU
1	E	240	PRO
1	A	118	ASN
1	A	133	LYS
1	A	239	VAL
1	B	239	VAL
1	C	118	ASN
1	C	133	LYS
1	C	239	VAL
1	C	240	PRO
1	D	118	ASN
1	D	239	VAL
1	D	269	ARG
1	E	239	VAL
1	D	120	HIS
1	E	133	LYS

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Mol	Chain	Res	Type
1	B	49	SER
1	B	59	PRO
1	D	133	LYS
1	A	340	ILE
1	B	202	ARG
1	B	243	ILE
1	B	261	ILE
1	D	160	ILE
1	D	203	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/310 (95%)	268 (91%)	27 (9%)	8	30
1	B	295/310 (95%)	272 (92%)	23 (8%)	11	35
1	C	295/310 (95%)	269 (91%)	26 (9%)	9	32
1	D	295/310 (95%)	264 (90%)	31 (10%)	6	24
1	E	295/310 (95%)	266 (90%)	29 (10%)	7	27
All	All	1475/1550 (95%)	1339 (91%)	136 (9%)	8	30

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	99	VAL
1	A	109	VAL
1	A	118	ASN
1	A	119	LEU
1	A	132	THR
1	A	137	LEU
1	A	162	ARG
1	A	164	LYS
1	A	200	LEU

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Mol	Chain	Res	Type
1	A	205	LYS
1	A	218	LEU
1	A	220	GLU
1	A	224	THR
1	A	234	SER
1	A	238	ASP
1	A	239	VAL
1	A	242	LEU
1	A	258	THR
1	A	269	ARG
1	A	284	SER
1	A	287	THR
1	A	293	VAL
1	A	294	LEU
1	A	297	ILE
1	A	315	PHE
1	A	341	MET
1	B	137	LEU
1	B	164	LYS
1	B	198	GLU
1	B	200	LEU
1	B	201	GLU
1	B	202	ARG
1	B	205	LYS
1	B	207	THR
1	B	220	GLU
1	B	234	SER
1	B	239	VAL
1	B	242	LEU
1	B	258	THR
1	B	263	ASP
1	B	265	VAL
1	B	269	ARG
1	B	283	VAL
1	B	287	THR
1	B	293	VAL
1	B	296	ILE
1	B	297	ILE
1	B	315	PHE
1	B	341	MET
1	C	62	ILE
1	C	85	LEU

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Mol	Chain	Res	Type
1	C	99	VAL
1	C	125	GLU
1	C	137	LEU
1	C	162	ARG
1	C	164	LYS
1	C	174	ILE
1	C	178	VAL
1	C	188	ILE
1	C	198	GLU
1	C	200	LEU
1	C	205	LYS
1	C	209	GLN
1	C	220	GLU
1	C	239	VAL
1	C	242	LEU
1	C	269	ARG
1	C	275	LEU
1	C	283	VAL
1	C	287	THR
1	C	293	VAL
1	C	297	ILE
1	C	302	MET
1	C	315	PHE
1	C	341	MET
1	D	40	ARG
1	D	99	VAL
1	D	118	ASN
1	D	119	LEU
1	D	123	GLU
1	D	128	SER
1	D	132	THR
1	D	135	CYS
1	D	150	VAL
1	D	152	GLU
1	D	164	LYS
1	D	178	VAL
1	D	183	VAL
1	D	184	LEU
1	D	198	GLU
1	D	200	LEU
1	D	201	GLU
1	D	205	LYS

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Mol	Chain	Res	Type
1	D	218	LEU
1	D	220	GLU
1	D	239	VAL
1	D	242	LEU
1	D	258	THR
1	D	263	ASP
1	D	283	VAL
1	D	287	THR
1	D	293	VAL
1	D	295	THR
1	D	297	ILE
1	D	315	PHE
1	D	341	MET
1	E	31	VAL
1	E	38	GLU
1	E	85	LEU
1	E	109	VAL
1	E	114	THR
1	E	118	ASN
1	E	125	GLU
1	E	137	LEU
1	E	162	ARG
1	E	164	LYS
1	E	192	ILE
1	E	195	LEU
1	E	198	GLU
1	E	200	LEU
1	E	202	ARG
1	E	205	LYS
1	E	220	GLU
1	E	226	TRP
1	E	239	VAL
1	E	242	LEU
1	E	247	THR
1	E	258	THR
1	E	269	ARG
1	E	277	ASP
1	E	287	THR
1	E	293	VAL
1	E	297	ILE
1	E	315	PHE
1	E	341	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	95	GLN
1	A	120	HIS
1	A	126	GLN
1	A	217	ASN
1	A	288	ASN
1	B	33	ASN
1	B	95	GLN
1	B	118	ASN
1	B	140	GLN
1	B	217	ASN
1	C	33	ASN
1	C	126	GLN
1	C	140	GLN
1	C	212	HIS
1	C	213	GLN
1	C	217	ASN
1	C	314	ASN
1	D	33	ASN
1	D	126	GLN
1	D	212	HIS
1	D	217	ASN
1	D	285	ASN
1	D	314	ASN
1	E	33	ASN
1	E	95	GLN
1	E	212	HIS
1	E	213	GLN
1	E	217	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	314/330 (95%)	0.41	33 (10%) 11 13	82, 149, 185, 198	0
1	B	314/330 (95%)	0.31	18 (5%) 29 24	83, 153, 195, 210	0
1	C	314/330 (95%)	0.43	32 (10%) 12 14	81, 151, 193, 207	0
1	D	314/330 (95%)	0.47	28 (8%) 15 16	80, 145, 179, 192	0
1	E	314/330 (95%)	0.29	22 (7%) 22 20	81, 145, 181, 193	0
All	All	1570/1650 (95%)	0.38	133 (8%) 16 17	80, 149, 188, 210	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	84	PRO	7.5
1	C	103	GLU	6.8
1	E	249	PRO	6.7
1	D	28	GLU	6.7
1	A	143	ILE	6.6
1	C	104	ASN	6.1
1	E	78	GLU	5.8
1	D	143	ILE	5.8
1	D	347	LYS	5.7
1	E	246	GLU	5.7
1	A	84	PRO	5.5
1	A	74	GLN	5.4
1	E	245	LYS	5.2
1	A	88	GLU	5.0
1	A	123	GLU	4.7
1	D	91	LEU	4.6
1	D	88	GLU	4.6
1	D	117	LYS	4.6
1	C	211	THR	4.5
1	E	100	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	84	PRO	4.5
1	C	76	VAL	4.5
1	E	250	TYR	4.4
1	B	75	ARG	4.3
1	C	198	GLU	4.3
1	A	43	LYS	4.1
1	C	197	GLU	4.1
1	A	72	VAL	4.0
1	D	103	GLU	4.0
1	D	344	TYR	3.9
1	E	101	PHE	3.9
1	A	91	LEU	3.9
1	D	43	LYS	3.8
1	C	208	VAL	3.7
1	A	142	LYS	3.6
1	B	36	ILE	3.6
1	A	114	THR	3.5
1	E	102	PHE	3.5
1	B	76	VAL	3.5
1	A	46	ASP	3.5
1	A	28	GLU	3.5
1	D	44	THR	3.4
1	A	294	LEU	3.4
1	E	106	VAL	3.4
1	D	87	LEU	3.4
1	B	77	GLY	3.4
1	E	82	ILE	3.4
1	A	85	LEU	3.4
1	A	117	LYS	3.4
1	C	273	SER	3.3
1	E	160	ILE	3.3
1	D	90	ILE	3.3
1	A	83	HIS	3.3
1	E	326	GLY	3.2
1	B	143	ILE	3.2
1	A	47	VAL	3.2
1	A	102	PHE	3.2
1	C	205	LYS	3.1
1	A	71	ASP	3.1
1	A	345	PHE	3.1
1	E	171	TYR	3.0
1	C	212	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	75	ARG	3.0
1	C	113	PHE	2.9
1	B	326	GLY	2.9
1	D	348	LYS	2.9
1	B	100	GLU	2.9
1	D	65	THR	2.9
1	A	298	ALA	2.9
1	A	201	GLU	2.9
1	C	101	PHE	2.8
1	A	144	GLY	2.8
1	C	204	GLU	2.8
1	A	161	ILE	2.8
1	A	212	HIS	2.7
1	E	83	HIS	2.7
1	C	102	PHE	2.7
1	D	298	ALA	2.7
1	A	297	ILE	2.7
1	C	146	VAL	2.7
1	D	42	PHE	2.7
1	D	345	PHE	2.7
1	C	301	PHE	2.7
1	B	273	SER	2.6
1	A	70	THR	2.6
1	B	194	VAL	2.6
1	C	62	ILE	2.6
1	C	73	VAL	2.6
1	C	249	PRO	2.6
1	D	257	HIS	2.5
1	B	78	GLU	2.5
1	A	299	THR	2.5
1	E	247	THR	2.5
1	B	73	VAL	2.5
1	B	28	GLU	2.5
1	D	209	GLN	2.5
1	E	335	GLY	2.4
1	C	245	LYS	2.4
1	D	161	ILE	2.4
1	E	208	VAL	2.4
1	C	64	ILE	2.4
1	C	311	TYR	2.4
1	D	78	GLU	2.4
1	E	205	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	123	GLU	2.3
1	B	64	ILE	2.3
1	C	30	GLU	2.3
1	B	241	PRO	2.3
1	A	73	VAL	2.3
1	C	326	GLY	2.3
1	C	250	TYR	2.3
1	C	31	VAL	2.2
1	C	314	ASN	2.2
1	C	194	VAL	2.2
1	A	65	THR	2.2
1	B	99	VAL	2.2
1	D	107	PHE	2.2
1	A	301	PHE	2.2
1	D	115	TYR	2.2
1	A	90	ILE	2.1
1	D	37	GLU	2.1
1	B	65	THR	2.1
1	C	29	ILE	2.1
1	E	296	ILE	2.1
1	E	339	VAL	2.1
1	B	124	SER	2.1
1	C	202	ARG	2.1
1	C	50	VAL	2.1
1	D	349	LYS	2.0
1	D	26	ASP	2.0
1	A	164	LYS	2.0
1	B	206	GLU	2.0
1	C	244	GLU	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 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(Å ²)	Q<0.9
2	MG	D	503	1/1	0.36	0.39	80,80,80,80	0
2	MG	E	502	1/1	0.78	0.14	56,56,56,56	0
2	MG	D	502	1/1	0.82	0.16	17,17,17,17	0
2	MG	A	401	1/1	0.82	0.08	75,75,75,75	0
2	MG	C	501	1/1	0.82	0.10	79,79,79,79	0
2	MG	B	502	1/1	0.86	0.22	58,58,58,58	0
2	MG	E	501	1/1	0.87	0.12	48,48,48,48	0
2	MG	A	402	1/1	0.87	0.09	45,45,45,45	0
2	MG	A	403	1/1	0.88	0.22	23,23,23,23	0
2	MG	A	404	1/1	0.89	0.09	88,88,88,88	0
2	MG	B	503	1/1	0.93	0.14	22,22,22,22	0
2	MG	C	502	1/1	0.94	0.08	47,47,47,47	0
2	MG	D	501	1/1	0.94	0.04	113,113,113,113	0
2	MG	B	501	1/1	0.96	0.03	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.