



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:18 PM GMT

PDB ID : 4EEB
Title : CorA coiled-coil mutant under Mg²⁺ absence
Authors : Pfoh, R.; Pai, E.F.
Deposited on : 2012-03-28
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

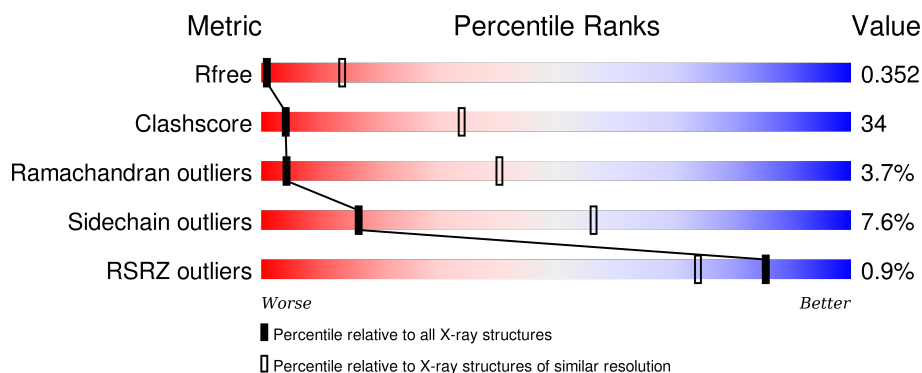
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	330	
1	C	330	
1	D	330	
1	E	330	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12988 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
1	A	314	Total	C	N	O	S	0	0	0
			2593	1688	418	478	9			
1	B	316	Total	C	N	O	S	0	0	0
			2606	1697	419	481	9			
1	C	314	Total	C	N	O	S	0	0	0
			2593	1688	418	478	9			
1	D	314	Total	C	N	O	S	0	0	0
			2593	1688	418	478	9			
1	E	314	Total	C	N	O	S	0	0	0
			2593	1688	418	478	9			

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 CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Cs 3 3	0	0
2	A	1	Total Cs 1 1	0	0
2	D	1	Total Cs 1 1	0	0
2	C	1	Total Cs 1 1	0	0
2	E	3	Total Cs 3 3	0	0

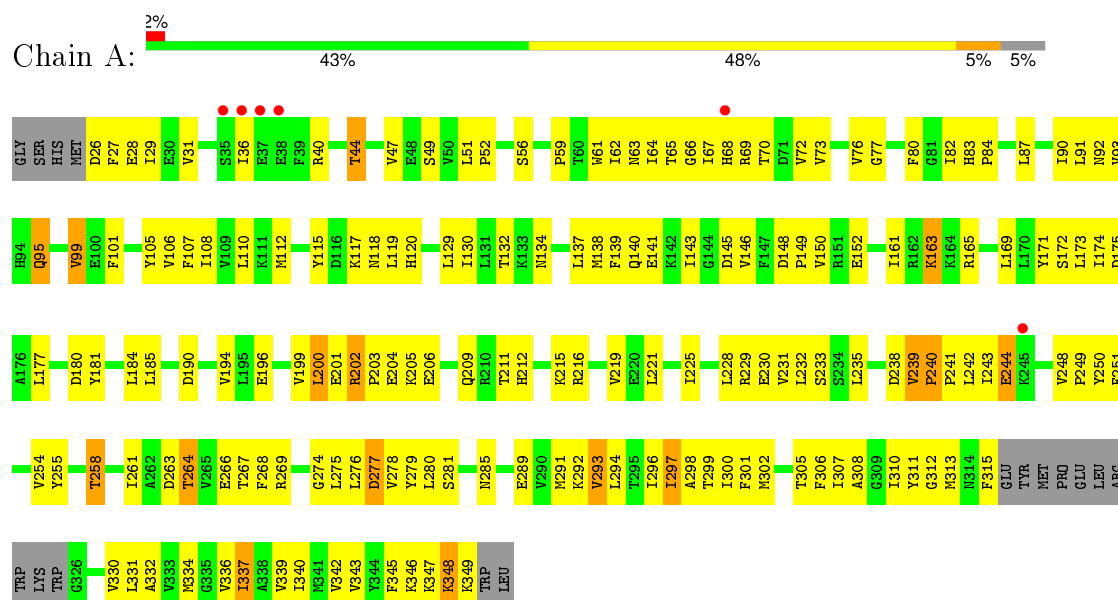
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

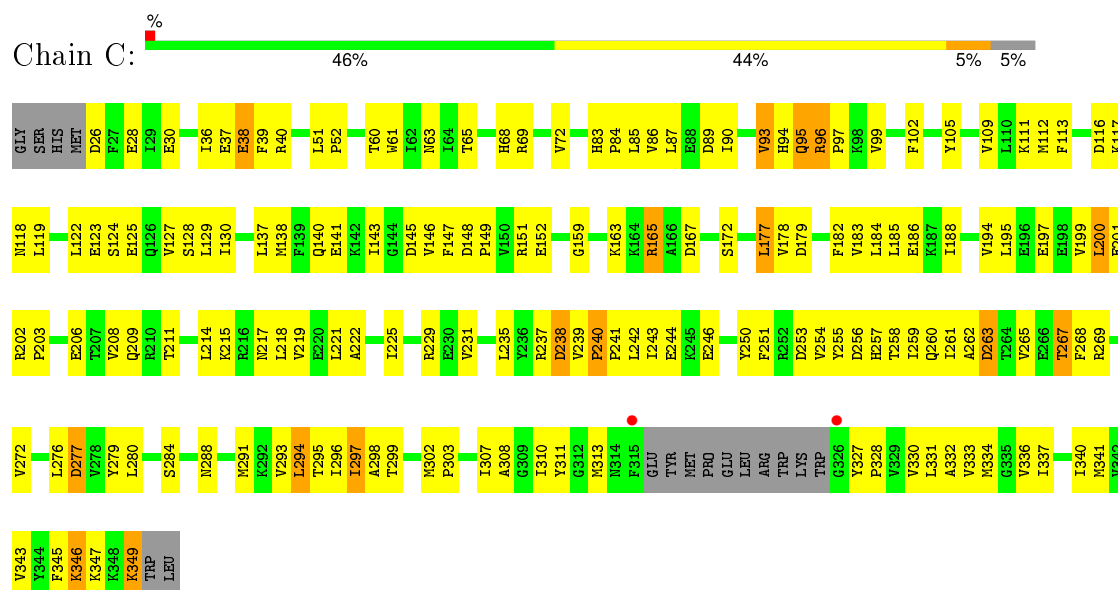
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

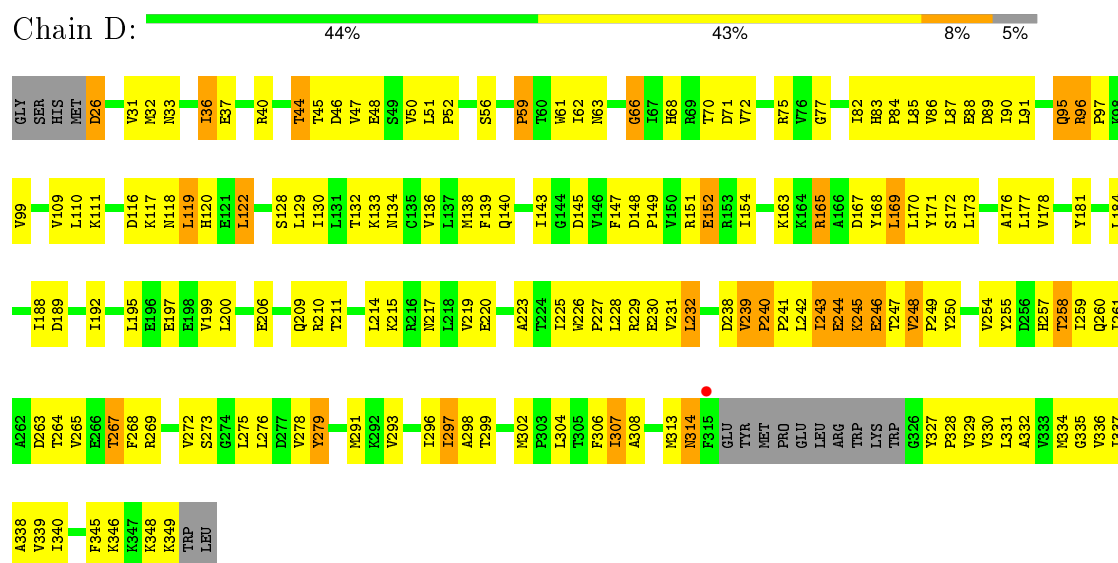
• Molecule 1: Magnesium transport protein CorA



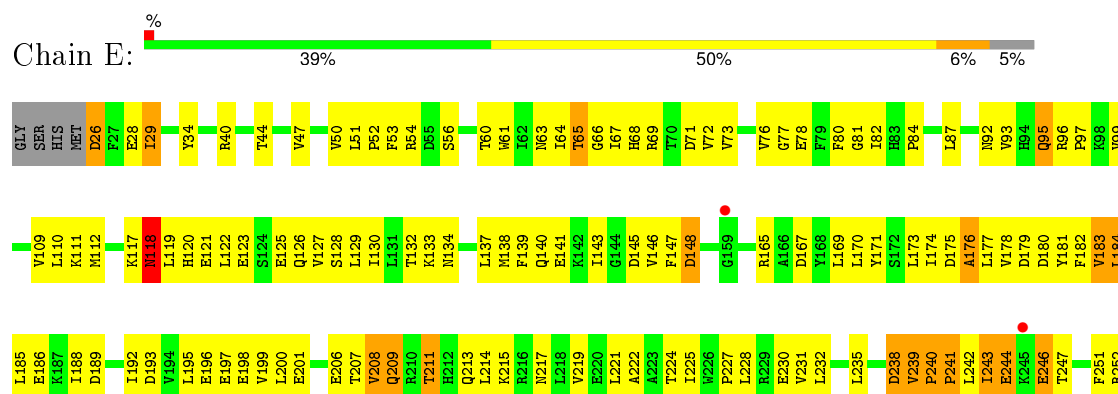
- Molecule 1: Magnesium transport protein CorA



- Molecule 1: Magnesium transport protein CorA



- Molecule 1: Magnesium transport protein CorA



ARG	TRP	LVS	TRP	G326	G327	P328	V329	V330	L331	A332	V333	M334	G335	V336	I337	A338	V339	I340	M341	V342	V343	V344	F345	K346	K347	K348	K349	TRP	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	125.60 Å 221.90 Å 106.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 3.80 19.89 – 3.80	Depositor EDS
% Data completeness (in resolution range)	80.4 (19.92-3.80) 80.4 (19.89-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.82 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.299 , 0.343 0.297 , 0.352	Depositor DCC
R_{free} test set	1189 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	121.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 24030 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12988	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/2646 (0.0%)	0.67	0/3588
1	B	0.62	0/2660	0.72	0/3609
1	C	0.68	0/2646	0.72	0/3588
1	D	0.66	0/2646	0.73	0/3588
1	E	0.58	0/2646	0.69	0/3588
All	All	0.63	1/13244 (0.0%)	0.71	0/17961

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	GLU	CD-OE2	5.12	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2593	0	2629	183	0
1	B	2606	0	2630	211	0
1	C	2593	0	2630	170	0
1	D	2593	0	2630	211	0
1	E	2593	0	2629	187	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	3	0	0	0	0
3	B	1	0	0	0	0
All	All	12988	0	13148	883	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 34.

All (883) 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:D:99:VAL:CG2	1:D:231:VAL:HG13	1.63	1.27
1:B:99:VAL:CG2	1:B:231:VAL:HG13	1.72	1.18
1:E:99:VAL:CG2	1:E:231:VAL:HG13	1.74	1.16
1:B:99:VAL:HG23	1:B:231:VAL:HG13	1.30	1.11
1:A:239:VAL:HG11	1:A:248:VAL:CG2	1.80	1.10
1:D:261:ILE:O	1:D:265:VAL:HG23	1.50	1.08
1:A:296:ILE:O	1:A:299:THR:HG22	1.55	1.07
1:E:255:TYR:O	1:E:258:THR:HG22	1.56	1.05
1:C:222:ALA:HB2	1:C:265:VAL:HG11	1.31	1.05
1:E:304:LEU:HD23	1:E:307:ILE:HD11	1.38	1.05
1:E:99:VAL:HG23	1:E:231:VAL:HG13	1.07	1.04
1:D:99:VAL:HG21	1:D:231:VAL:HG13	1.33	1.04
1:A:211:THR:HG21	1:A:276:LEU:HD13	1.41	1.01
1:B:255:TYR:O	1:B:258:THR:HG22	1.61	1.00
1:A:255:TYR:O	1:A:258:THR:HG22	1.59	0.99
1:A:215:LYS:O	1:A:219:VAL:HG23	1.64	0.95
1:C:211:THR:HG21	1:C:276:LEU:HD13	1.48	0.94
1:D:331:LEU:HD23	1:D:334:MET:CE	1.98	0.93
1:E:99:VAL:CG2	1:E:231:VAL:CG1	2.46	0.93
1:B:215:LYS:O	1:B:219:VAL:HG23	1.70	0.92
1:D:99:VAL:HG23	1:D:231:VAL:HG13	1.51	0.91
1:A:313:MET:HE1	1:B:308:ALA:O	1.69	0.91
1:B:99:VAL:CG2	1:B:231:VAL:CG1	2.49	0.91
1:B:307:ILE:HD11	1:B:334:MET:HG2	1.54	0.90
1:D:296:ILE:HA	1:D:299:THR:HG22	1.54	0.90
1:E:82:ILE:HD13	1:E:130:ILE:HD13	1.54	0.90
1:D:199:VAL:HG13	1:D:279:TYR:HB2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG11	1:A:248:VAL:HG21	1.53	0.89
1:B:182:PHE:HA	1:B:185:LEU:HD12	1.54	0.89
1:B:313:MET:HA	1:B:313:MET:HE2	1.55	0.88
1:A:47:VAL:HG21	1:A:72:VAL:HG13	1.55	0.88
1:A:232:LEU:HD23	1:A:235:LEU:HD22	1.54	0.87
1:E:64:ILE:HD13	1:E:139:PHE:CE1	2.09	0.87
1:B:280:LEU:HD23	1:C:280:LEU:HD21	1.57	0.87
1:E:99:VAL:HG23	1:E:231:VAL:CG1	1.99	0.85
1:D:313:MET:HE1	1:E:308:ALA:O	1.76	0.85
1:A:239:VAL:HG11	1:A:248:VAL:HG22	1.56	0.85
1:E:65:THR:HG21	1:E:143:ILE:HD13	1.57	0.85
1:C:167:ASP:HB2	1:C:242:LEU:HD23	1.56	0.85
1:D:122:LEU:HD22	1:D:217:ASN:ND2	1.92	0.84
1:A:336:VAL:O	1:A:340:ILE:HG23	1.77	0.84
1:C:243:ILE:HD12	1:C:246:GLU:HB2	1.59	0.84
1:B:240:PRO:HB2	1:B:241:PRO:CD	2.09	0.82
1:A:347:LYS:O	1:A:348:LYS:HB2	1.78	0.82
1:B:242:LEU:HD21	1:B:251:PHE:CE1	2.14	0.82
1:C:331:LEU:HD23	1:C:334:MET:HE2	1.60	0.82
1:D:177:LEU:HD21	1:D:181:TYR:HE1	1.44	0.82
1:E:331:LEU:HD23	1:E:334:MET:CE	2.09	0.82
1:B:225:ILE:HD13	1:B:265:VAL:HG21	1.62	0.82
1:B:88:GLU:HA	1:B:91:LEU:HD12	1.62	0.81
1:C:296:ILE:HA	1:C:299:THR:HG22	1.61	0.81
1:A:200:LEU:HD22	1:B:209:GLN:HG2	1.63	0.81
1:D:165:ARG:HH12	1:D:243:ILE:HD13	1.46	0.80
1:A:63:ASN:HB2	1:A:138:MET:HE2	1.63	0.80
1:D:184:LEU:O	1:D:188:ILE:HD12	1.81	0.80
1:A:47:VAL:CG2	1:A:72:VAL:HG13	2.11	0.80
1:E:29:ILE:HG21	1:E:50:VAL:HG11	1.63	0.80
1:A:221:LEU:O	1:A:225:ILE:HD12	1.82	0.80
1:E:184:LEU:HD12	1:E:184:LEU:O	1.82	0.80
1:D:122:LEU:HD22	1:D:217:ASN:HD22	1.47	0.79
1:C:130:ILE:HB	1:C:137:LEU:HD12	1.64	0.79
1:C:255:TYR:O	1:C:258:THR:HG22	1.82	0.79
1:E:335:GLY:O	1:E:339:VAL:HG23	1.81	0.78
1:D:239:VAL:HG11	1:D:248:VAL:CG2	2.13	0.78
1:C:65:THR:HG21	1:C:143:ILE:HG12	1.65	0.78
1:B:51:LEU:HD22	1:B:79:PHE:CD2	2.18	0.78
1:C:313:MET:HE3	1:D:308:ALA:HB1	1.66	0.78
1:B:177:LEU:HD21	1:B:181:TYR:HE1	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:O	1:D:239:VAL:HG23	1.82	0.77
1:D:47:VAL:HG22	1:D:51:LEU:HD21	1.66	0.77
1:D:109:VAL:O	1:D:110:LEU:HD23	1.84	0.77
1:C:256:ASP:HA	1:C:259:ILE:HD12	1.67	0.77
1:C:331:LEU:HD23	1:C:334:MET:CE	2.15	0.76
1:C:194:VAL:HG12	1:C:194:VAL:O	1.84	0.76
1:E:76:VAL:HG13	1:E:80:PHE:CD2	2.20	0.76
1:D:313:MET:HA	1:D:313:MET:HE2	1.67	0.76
1:C:299:THR:HG21	1:C:345:PHE:CZ	2.20	0.76
1:E:177:LEU:HD23	1:E:177:LEU:C	2.06	0.75
1:B:131:LEU:HD12	1:B:135:CYS:O	1.85	0.75
1:C:302:MET:HE2	1:D:297:ILE:HG23	1.67	0.75
1:E:165:ARG:HH12	1:E:243:ILE:HD13	1.51	0.75
1:C:310:ILE:O	1:C:313:MET:HG2	1.87	0.75
1:B:222:ALA:HB2	1:B:265:VAL:HG11	1.69	0.74
1:E:215:LYS:O	1:E:219:VAL:HG23	1.88	0.74
1:D:128:SER:O	1:D:129:LEU:HD23	1.87	0.74
1:C:99:VAL:CG2	1:C:231:VAL:HG13	2.17	0.74
1:A:70:THR:HG22	1:A:91:LEU:HD22	1.68	0.74
1:C:302:MET:CE	1:D:297:ILE:HG23	2.17	0.74
1:E:296:ILE:HG22	1:E:345:PHE:CE1	2.23	0.74
1:D:61:TRP:HB2	1:D:169:LEU:HD21	1.69	0.73
1:D:31:VAL:HG22	1:D:62:ILE:HG12	1.70	0.73
1:D:169:LEU:O	1:D:169:LEU:HD12	1.89	0.73
1:C:83:HIS:NE2	1:C:85:LEU:HD12	2.04	0.72
1:C:243:ILE:HD12	1:C:246:GLU:CB	2.18	0.72
1:C:313:MET:HE3	1:D:308:ALA:O	1.88	0.72
1:D:255:TYR:O	1:D:258:THR:HB	1.90	0.72
1:D:177:LEU:HD21	1:D:181:TYR:CE1	2.24	0.72
1:B:29:ILE:HB	1:B:44:THR:HG23	1.71	0.72
1:A:174:ILE:HG21	1:A:232:LEU:HD21	1.71	0.72
1:B:242:LEU:CD2	1:B:251:PHE:HE1	2.03	0.72
1:D:243:ILE:HD12	1:D:246:GLU:HB3	1.72	0.72
1:D:165:ARG:NH1	1:D:243:ILE:HD13	2.04	0.71
1:B:245:LYS:O	1:B:246:GLU:HB2	1.89	0.71
1:A:67:ILE:HD11	1:A:93:VAL:CG1	2.20	0.71
1:E:122:LEU:HD22	1:E:217:ASN:HD22	1.56	0.71
1:A:65:THR:HG21	1:A:143:ILE:HD13	1.71	0.71
1:E:239:VAL:HG23	1:E:239:VAL:O	1.91	0.71
1:A:269:ARG:NH1	1:E:270:ASP:OD1	2.23	0.70
1:D:99:VAL:CG2	1:D:231:VAL:CG1	2.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:HIS:ND1	1:B:84:PRO:HD2	2.07	0.70
1:A:36:ILE:HD13	1:A:163:LYS:HG3	1.73	0.70
1:B:110:LEU:CD1	1:B:177:LEU:HD13	2.22	0.70
1:D:331:LEU:HD23	1:D:334:MET:HE2	1.74	0.70
1:D:297:ILE:HG22	1:D:298:ALA:N	2.07	0.70
1:D:331:LEU:HD23	1:D:334:MET:HE3	1.73	0.69
1:B:70:THR:HG22	1:B:91:LEU:HD22	1.74	0.69
1:E:331:LEU:HD23	1:E:334:MET:HE3	1.73	0.69
1:B:177:LEU:HD21	1:B:181:TYR:CE1	2.28	0.69
1:C:296:ILE:HD12	1:C:297:ILE:N	2.07	0.69
1:B:65:THR:HG21	1:B:143:ILE:HD13	1.74	0.69
1:B:99:VAL:HG22	1:B:231:VAL:HG13	1.71	0.69
1:B:347:LYS:O	1:B:348:LYS:HB2	1.92	0.69
1:B:82:ILE:HD13	1:B:130:ILE:HD13	1.73	0.69
1:B:295:THR:HG23	1:C:294:LEU:HG	1.74	0.69
1:E:130:ILE:HB	1:E:137:LEU:HD12	1.74	0.68
1:E:84:PRO:HA	1:E:87:LEU:HD12	1.75	0.68
1:B:106:VAL:O	1:B:130:ILE:HG23	1.92	0.68
1:B:313:MET:CE	1:C:311:TYR:HB2	2.24	0.68
1:A:313:MET:CE	1:B:308:ALA:O	2.42	0.68
1:D:335:GLY:O	1:D:339:VAL:HG23	1.94	0.68
1:C:225:ILE:HD12	1:C:265:VAL:HG21	1.74	0.67
1:B:242:LEU:CD2	1:B:251:PHE:CE1	2.76	0.67
1:C:215:LYS:O	1:C:219:VAL:HG23	1.95	0.67
1:B:65:THR:HG21	1:B:143:ILE:CD1	2.25	0.67
1:D:313:MET:CE	1:E:308:ALA:O	2.42	0.67
1:B:299:THR:HA	1:C:297:ILE:HG21	1.76	0.67
1:D:296:ILE:HA	1:D:299:THR:CG2	2.24	0.67
1:B:47:VAL:O	1:B:50:VAL:HG22	1.94	0.67
1:D:177:LEU:CD2	1:D:181:TYR:HE1	2.06	0.67
1:D:334:MET:O	1:D:338:ALA:HB2	1.94	0.66
1:E:256:ASP:HA	1:E:259:ILE:HD12	1.77	0.66
1:E:333:VAL:O	1:E:337:ILE:HG23	1.95	0.66
1:E:296:ILE:HA	1:E:299:THR:HG22	1.77	0.66
1:B:110:LEU:HD13	1:B:177:LEU:HD13	1.77	0.66
1:C:165:ARG:HH12	1:C:243:ILE:HD13	1.60	0.66
1:B:36:ILE:HG23	1:B:37:GLU:HG3	1.77	0.66
1:B:313:MET:CE	1:C:308:ALA:O	2.44	0.66
1:D:84:PRO:HA	1:D:87:LEU:HD12	1.78	0.66
1:D:33:ASN:ND2	1:D:59:PRO:O	2.29	0.66
1:B:242:LEU:O	1:B:244:GLU:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ILE:HB	1:B:137:LEU:HD12	1.77	0.66
1:B:240:PRO:HB2	1:B:241:PRO:HD3	1.77	0.65
1:D:239:VAL:HG11	1:D:248:VAL:HG23	1.79	0.65
1:E:296:ILE:CD1	1:E:297:ILE:HD12	2.26	0.65
1:B:173:LEU:O	1:B:176:ALA:HB3	1.96	0.65
1:D:136:VAL:HG11	1:D:173:LEU:CD1	2.25	0.65
1:E:184:LEU:O	1:E:188:ILE:HD12	1.96	0.65
1:B:166:ALA:O	1:B:169:LEU:HB3	1.95	0.65
1:D:195:LEU:HD21	1:D:211:THR:HA	1.77	0.65
1:B:195:LEU:O	1:B:199:VAL:HG23	1.97	0.65
1:A:331:LEU:HA	1:A:334:MET:HE2	1.77	0.65
1:E:61:TRP:HB2	1:E:169:LEU:HD21	1.79	0.65
1:B:61:TRP:C	1:B:61:TRP:CD1	2.70	0.64
1:D:296:ILE:HG22	1:D:345:PHE:CZ	2.32	0.64
1:C:328:PRO:HA	1:C:331:LEU:HD12	1.78	0.64
1:D:178:VAL:HG21	1:D:254:VAL:CG1	2.26	0.64
1:A:87:LEU:HD23	1:A:90:ILE:HD12	1.80	0.64
1:B:131:LEU:HD11	1:B:166:ALA:HB1	1.79	0.64
1:B:86:VAL:HG13	1:B:107:PHE:CE2	2.30	0.64
1:B:27:PHE:CZ	1:B:72:VAL:HG21	2.33	0.64
1:C:221:LEU:HD23	1:C:265:VAL:HG22	1.78	0.64
1:D:170:LEU:O	1:D:171:TYR:C	2.35	0.64
1:B:247:THR:HA	1:B:250:TYR:HD2	1.60	0.64
1:A:27:PHE:CD1	1:A:69:ARG:HG3	2.33	0.64
1:E:195:LEU:O	1:E:199:VAL:HG23	1.97	0.64
1:A:56:SER:O	1:A:134:ASN:ND2	2.30	0.64
1:D:331:LEU:CD2	1:D:334:MET:CE	2.74	0.64
1:D:177:LEU:C	1:D:177:LEU:HD23	2.18	0.64
1:A:36:ILE:CD1	1:A:163:LYS:HG3	2.28	0.63
1:B:83:HIS:HE2	1:B:85:LEU:HD12	1.62	0.63
1:D:299:THR:HA	1:E:297:ILE:HG21	1.80	0.63
1:E:29:ILE:CG2	1:E:50:VAL:HG11	2.29	0.63
1:A:209:GLN:HG2	1:E:200:LEU:HD22	1.81	0.63
1:E:65:THR:HG21	1:E:143:ILE:CD1	2.29	0.63
1:B:278:VAL:HA	1:C:276:LEU:HD21	1.81	0.63
1:A:61:TRP:HB2	1:A:169:LEU:HD21	1.80	0.63
1:C:333:VAL:HA	1:C:336:VAL:HB	1.80	0.63
1:A:65:THR:HG21	1:A:143:ILE:CD1	2.28	0.62
1:A:177:LEU:O	1:A:180:ASP:HB3	1.98	0.62
1:D:32:MET:HE1	1:D:154:ILE:HB	1.81	0.62
1:E:122:LEU:HD22	1:E:217:ASN:ND2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HA	1:B:90:ILE:HD12	1.81	0.62
1:D:267:THR:HG22	1:D:268:PHE:N	2.13	0.62
1:A:185:LEU:HD11	1:A:261:ILE:HG23	1.79	0.62
1:A:150:VAL:HG11	1:A:173:LEU:HD23	1.81	0.62
1:D:296:ILE:CA	1:D:299:THR:HG22	2.28	0.61
1:B:211:THR:HG23	1:B:275:LEU:HD23	1.82	0.61
1:B:222:ALA:HA	1:B:225:ILE:HD12	1.83	0.61
1:E:97:PRO:HB3	1:E:228:LEU:HD12	1.83	0.61
1:B:113:PHE:CE1	1:B:124:SER:HB3	2.35	0.61
1:E:26:ASP:N	1:E:68:HIS:HE2	1.99	0.61
1:C:332:ALA:O	1:C:336:VAL:HG23	2.00	0.61
1:E:232:LEU:HD11	1:E:254:VAL:HG12	1.82	0.61
1:E:199:VAL:HG13	1:E:279:TYR:HB2	1.82	0.61
1:B:185:LEU:HD11	1:B:261:ILE:HG23	1.83	0.60
1:B:298:ALA:CB	1:C:294:LEU:HD21	2.30	0.60
1:D:199:VAL:HG13	1:D:279:TYR:CB	2.30	0.60
1:C:313:MET:CE	1:D:308:ALA:O	2.48	0.60
1:C:218:LEU:HD23	1:C:269:ARG:HA	1.83	0.60
1:A:80:PHE:CZ	1:A:137:LEU:HD21	2.36	0.60
1:A:235:LEU:HD23	1:A:251:PHE:CE2	2.37	0.60
1:B:242:LEU:HD21	1:B:251:PHE:CZ	2.37	0.60
1:A:289:GLU:O	1:A:293:VAL:HG23	2.00	0.60
1:A:165:ARG:HH12	1:A:243:ILE:HD13	1.67	0.60
1:A:299:THR:HG23	1:A:300:ILE:HG23	1.82	0.60
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.84	0.60
1:C:83:HIS:ND1	1:C:84:PRO:HD2	2.17	0.60
1:D:242:LEU:O	1:D:243:ILE:C	2.40	0.60
1:C:99:VAL:HG22	1:C:231:VAL:HG13	1.82	0.60
1:E:232:LEU:CD1	1:E:254:VAL:HG12	2.31	0.60
1:A:313:MET:HA	1:A:313:MET:HE2	1.84	0.60
1:C:240:PRO:HB2	1:C:241:PRO:CD	2.32	0.60
1:A:63:ASN:CB	1:A:138:MET:HE2	2.31	0.59
1:E:240:PRO:HB2	1:E:241:PRO:CD	2.32	0.59
1:A:301:PHE:O	1:A:305:THR:OG1	2.10	0.59
1:C:302:MET:HE2	1:D:297:ILE:CG2	2.31	0.59
1:B:310:ILE:O	1:B:313:MET:HG2	2.03	0.59
1:D:291:MET:HE1	1:E:291:MET:HG2	1.84	0.59
1:A:110:LEU:HD22	1:A:228:LEU:HD13	1.83	0.59
1:E:171:TYR:HE1	1:E:254:VAL:HG23	1.67	0.59
1:A:64:ILE:HD12	1:A:139:PHE:CE1	2.37	0.59
1:B:261:ILE:O	1:B:265:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HG22	1:B:298:ALA:N	2.16	0.59
1:C:311:TYR:HE2	1:C:330:VAL:HG21	1.68	0.59
1:D:184:LEU:O	1:D:188:ILE:CD1	2.51	0.59
1:C:267:THR:HG22	1:C:268:PHE:N	2.17	0.59
1:C:148:ASP:N	1:C:149:PRO:HD2	2.17	0.59
1:C:296:ILE:HA	1:C:299:THR:CG2	2.30	0.59
1:A:339:VAL:HA	1:A:342:VAL:HG23	1.85	0.59
1:B:238:ASP:O	1:B:239:VAL:HG22	2.03	0.58
1:E:231:VAL:O	1:E:235:LEU:HD13	2.03	0.58
1:A:200:LEU:HD22	1:B:209:GLN:CG	2.32	0.58
1:E:268:PHE:O	1:E:272:VAL:HG23	2.03	0.58
1:C:222:ALA:HB2	1:C:265:VAL:CG1	2.20	0.58
1:D:299:THR:HG21	1:D:345:PHE:CZ	2.38	0.58
1:D:245:LYS:O	1:D:246:GLU:HG2	2.03	0.58
1:E:66:GLY:HA2	1:E:141:GLU:O	2.03	0.58
1:A:291:MET:HB3	1:B:290:VAL:HG11	1.85	0.58
1:C:97:PRO:HA	1:C:109:VAL:O	2.03	0.58
1:E:296:ILE:HD12	1:E:297:ILE:HD12	1.85	0.58
1:B:65:THR:HG21	1:B:143:ILE:CG1	2.33	0.58
1:A:115:TYR:OH	1:A:120:HIS:HA	2.04	0.58
1:B:99:VAL:HG22	1:B:231:VAL:CG1	2.29	0.58
1:A:110:LEU:HD22	1:A:228:LEU:CD1	2.34	0.58
1:C:165:ARG:NH1	1:C:243:ILE:HD13	2.18	0.57
1:C:260:GLN:HA	1:D:96:ARG:HH21	1.69	0.57
1:C:60:THR:CG2	1:C:61:TRP:N	2.66	0.57
1:B:138:MET:SD	1:B:147:PHE:CE2	2.97	0.57
1:D:330:VAL:O	1:D:334:MET:HG3	2.04	0.57
1:E:313:MET:HA	1:E:313:MET:HE2	1.87	0.57
1:B:178:VAL:HG21	1:B:254:VAL:HG12	1.86	0.57
1:D:122:LEU:CD2	1:D:217:ASN:HD22	2.15	0.57
1:D:82:ILE:HG22	1:D:87:LEU:HG	1.86	0.57
1:C:63:ASN:OD1	1:C:138:MET:HE2	2.03	0.57
1:B:240:PRO:CB	1:B:241:PRO:CD	2.82	0.57
1:E:185:LEU:O	1:E:186:GLU:C	2.42	0.57
1:E:252:ARG:O	1:E:255:TYR:HB3	2.04	0.57
1:A:171:TYR:CE1	1:A:250:TYR:HB3	2.40	0.57
1:D:225:ILE:HD13	1:D:261:ILE:CG2	2.34	0.57
1:D:171:TYR:O	1:D:172:SER:C	2.41	0.57
1:E:77:GLY:CA	1:E:87:LEU:HD21	2.34	0.57
1:D:306:PHE:CD1	1:D:307:ILE:HG23	2.40	0.57
1:B:177:LEU:CD2	1:B:181:TYR:HE1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:LEU:HA	1:E:188:ILE:HD12	1.86	0.57
1:E:329:VAL:O	1:E:333:VAL:HG23	2.05	0.57
1:A:31:VAL:HG22	1:A:62:ILE:HG23	1.87	0.57
1:B:248:VAL:HG12	1:B:249:PRO:CD	2.35	0.57
1:E:118:ASN:OD1	1:E:119:LEU:N	2.37	0.57
1:E:242:LEU:O	1:E:243:ILE:C	2.42	0.56
1:B:313:MET:HA	1:B:313:MET:CE	2.33	0.56
1:B:169:LEU:O	1:B:172:SER:N	2.38	0.56
1:E:225:ILE:HD12	1:E:265:VAL:HG21	1.87	0.56
1:E:165:ARG:NH1	1:E:243:ILE:HD13	2.19	0.56
1:C:240:PRO:HB2	1:C:241:PRO:HD3	1.87	0.56
1:A:112:MET:SD	1:A:146:VAL:HG13	2.46	0.56
1:B:112:MET:CE	1:B:127:VAL:HG21	2.35	0.56
1:A:298:ALA:HA	1:E:302:MET:HE2	1.87	0.56
1:D:297:ILE:CG2	1:D:298:ALA:N	2.68	0.56
1:B:234:SER:O	1:B:238:ASP:HB2	2.05	0.56
1:D:71:ASP:N	1:D:71:ASP:OD1	2.39	0.56
1:E:235:LEU:HD23	1:E:251:PHE:CD2	2.41	0.56
1:D:47:VAL:HB	1:D:72:VAL:HG13	1.88	0.56
1:D:118:ASN:O	1:D:120:HIS:CE1	2.59	0.56
1:A:201:GLU:C	1:A:203:PRO:HD3	2.27	0.56
1:D:48:GLU:OE2	1:D:75:ARG:NE	2.38	0.56
1:B:247:THR:HG22	1:B:250:TYR:HB2	1.87	0.56
1:C:336:VAL:O	1:C:340:ILE:HG23	2.06	0.56
1:D:229:ARG:HA	1:D:258:THR:CG2	2.36	0.55
1:B:248:VAL:HG12	1:B:249:PRO:HD3	1.87	0.55
1:E:225:ILE:CD1	1:E:265:VAL:HG21	2.37	0.55
1:D:227:PRO:O	1:D:228:LEU:C	2.41	0.55
1:E:109:VAL:O	1:E:110:LEU:HD23	2.05	0.55
1:B:119:LEU:O	1:B:120:HIS:C	2.44	0.55
1:B:185:LEU:HD11	1:B:261:ILE:CG2	2.35	0.55
1:B:83:HIS:NE2	1:B:85:LEU:HD12	2.21	0.55
1:A:331:LEU:HD23	1:A:334:MET:CE	2.36	0.55
1:C:113:PHE:CE1	1:C:124:SER:HB3	2.40	0.55
1:D:165:ARG:NH1	1:D:243:ILE:HG21	2.20	0.55
1:B:65:THR:HG21	1:B:143:ILE:HG12	1.88	0.55
1:C:295:THR:CG2	1:D:293:VAL:HG11	2.36	0.55
1:C:147:PHE:O	1:C:151:ARG:HG3	2.07	0.55
1:B:229:ARG:HH11	1:B:259:ILE:HG23	1.71	0.55
1:B:300:ILE:HG22	1:B:341:MET:HG3	1.89	0.55
1:B:335:GLY:O	1:B:339:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LYS:O	1:A:119:LEU:N	2.39	0.55
1:A:248:VAL:N	1:A:249:PRO:HD2	2.22	0.55
1:E:306:PHE:HD1	1:E:307:ILE:HG23	1.72	0.55
1:C:36:ILE:HG23	1:C:37:GLU:HG3	1.88	0.55
1:A:291:MET:HE3	1:B:290:VAL:CG1	2.37	0.55
1:D:240:PRO:HB2	1:D:241:PRO:CD	2.36	0.55
1:A:66:GLY:N	1:A:140:GLN:O	2.40	0.55
1:D:296:ILE:O	1:D:299:THR:HG22	2.07	0.55
1:C:194:VAL:CG1	1:C:194:VAL:O	2.54	0.55
1:A:70:THR:HG22	1:A:91:LEU:CD2	2.37	0.55
1:D:275:LEU:O	1:D:278:VAL:N	2.37	0.55
1:A:47:VAL:HG21	1:A:72:VAL:CG1	2.33	0.55
1:C:63:ASN:HA	1:C:138:MET:HB3	1.89	0.55
1:E:338:ALA:O	1:E:342:VAL:HG23	2.06	0.55
1:D:225:ILE:HD13	1:D:261:ILE:HG22	1.89	0.54
1:C:295:THR:HG21	1:D:293:VAL:HG11	1.89	0.54
1:A:63:ASN:HB2	1:A:138:MET:CE	2.35	0.54
1:C:200:LEU:HD22	1:D:209:GLN:HG3	1.88	0.54
1:E:51:LEU:CD2	1:E:76:VAL:HG22	2.36	0.54
1:B:136:VAL:HG11	1:B:173:LEU:CD1	2.37	0.54
1:D:296:ILE:HD12	1:D:297:ILE:N	2.22	0.54
1:B:296:ILE:HA	1:B:299:THR:HG22	1.90	0.54
1:D:229:ARG:HA	1:D:258:THR:HG21	1.89	0.54
1:B:112:MET:HE2	1:B:127:VAL:HG21	1.90	0.54
1:C:296:ILE:O	1:C:299:THR:HG22	2.07	0.54
1:E:192:ILE:O	1:E:193:ASP:C	2.46	0.54
1:A:239:VAL:HG12	1:A:242:LEU:CD1	2.37	0.54
1:D:83:HIS:ND1	1:D:84:PRO:HD2	2.23	0.54
1:B:225:ILE:CG2	1:B:262:ALA:HB2	2.38	0.54
1:B:313:MET:HE3	1:C:308:ALA:O	2.05	0.54
1:A:61:TRP:HZ2	1:A:138:MET:HE1	1.73	0.54
1:C:130:ILE:CB	1:C:137:LEU:HD12	2.35	0.54
1:B:131:LEU:HD13	1:B:136:VAL:CG2	2.38	0.54
1:E:47:VAL:HB	1:E:72:VAL:HG13	1.88	0.54
1:B:263:ASP:CB	1:C:96:ARG:NH2	2.70	0.54
1:B:201:GLU:C	1:B:203:PRO:HD3	2.28	0.54
1:B:225:ILE:HG22	1:B:262:ALA:HB2	1.89	0.54
1:D:110:LEU:HD13	1:D:177:LEU:HD13	1.90	0.54
1:A:87:LEU:HD23	1:A:90:ILE:CD1	2.38	0.54
1:A:36:ILE:HD13	1:A:163:LYS:CG	2.38	0.54
1:D:272:VAL:O	1:D:275:LEU:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ILE:HG23	1:C:214:LEU:HD11	1.89	0.54
1:C:93:VAL:HG23	1:C:94:HIS:CE1	2.42	0.54
1:B:313:MET:HE1	1:C:308:ALA:O	2.07	0.53
1:D:313:MET:CA	1:D:313:MET:HE2	2.36	0.53
1:B:296:ILE:C	1:B:296:ILE:HD12	2.28	0.53
1:A:190:ASP:O	1:A:194:VAL:HG23	2.09	0.53
1:D:148:ASP:N	1:D:149:PRO:HD2	2.23	0.53
1:A:148:ASP:O	1:A:152:GLU:HG2	2.08	0.53
1:D:215:LYS:O	1:D:219:VAL:HG23	2.09	0.53
1:D:122:LEU:HD21	1:D:220:GLU:OE1	2.07	0.53
1:A:209:GLN:CG	1:E:200:LEU:HD22	2.39	0.53
1:E:227:PRO:O	1:E:230:GLU:N	2.42	0.53
1:D:260:GLN:HE22	1:E:95:GLN:HA	1.73	0.53
1:A:77:GLY:HA3	1:A:87:LEU:HD11	1.90	0.53
1:C:260:GLN:O	1:C:263:ASP:HB2	2.08	0.53
1:D:248:VAL:HG12	1:D:249:PRO:CD	2.38	0.53
1:D:51:LEU:N	1:D:52:PRO:HD2	2.24	0.53
1:A:291:MET:CE	1:B:290:VAL:HG12	2.38	0.53
1:E:109:VAL:HG11	1:E:126:GLN:OE1	2.09	0.53
1:E:64:ILE:CD1	1:E:139:PHE:CE1	2.89	0.53
1:C:36:ILE:HD13	1:C:163:LYS:HG3	1.91	0.53
1:A:294:LEU:CD2	1:B:294:LEU:HD11	2.38	0.53
1:E:300:ILE:O	1:E:304:LEU:HD12	2.09	0.53
1:C:211:THR:CG2	1:C:276:LEU:HD13	2.31	0.53
1:D:177:LEU:CD2	1:D:181:TYR:CE1	2.86	0.53
1:C:148:ASP:O	1:C:152:GLU:HG2	2.08	0.53
1:B:238:ASP:C	1:B:239:VAL:HG22	2.29	0.53
1:C:102:PHE:CG	1:C:105:TYR:CE1	2.97	0.53
1:B:216:ARG:O	1:B:219:VAL:HB	2.08	0.53
1:D:239:VAL:O	1:D:239:VAL:CG2	2.53	0.53
1:C:296:ILE:CA	1:C:299:THR:HG22	2.35	0.53
1:A:83:HIS:ND1	1:A:84:PRO:HD2	2.24	0.53
1:B:222:ALA:HB2	1:B:265:VAL:CG1	2.37	0.53
1:A:36:ILE:HD13	1:A:163:LYS:HA	1.91	0.53
1:A:199:VAL:HG13	1:A:279:TYR:HA	1.91	0.53
1:B:110:LEU:HD12	1:B:177:LEU:HD13	1.90	0.52
1:E:60:THR:HG22	1:E:61:TRP:N	2.25	0.52
1:C:93:VAL:HG23	1:C:94:HIS:NE2	2.24	0.52
1:D:178:VAL:HG21	1:D:254:VAL:HG12	1.90	0.52
1:B:67:ILE:HG23	1:B:140:GLN:O	2.09	0.52
1:C:311:TYR:CE2	1:C:330:VAL:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ARG:HG3	1:C:258:THR:HG23	1.91	0.52
1:B:178:VAL:HG21	1:B:254:VAL:CG1	2.39	0.52
1:C:183:VAL:HG13	1:C:186:GLU:OE2	2.09	0.52
1:E:296:ILE:HD11	1:E:297:ILE:HD12	1.91	0.52
1:E:307:ILE:HA	1:E:310:ILE:HD13	1.91	0.52
1:D:250:TYR:O	1:D:254:VAL:HG23	2.10	0.52
1:D:132:THR:O	1:D:132:THR:HG23	2.10	0.52
1:C:185:LEU:HD11	1:C:261:ILE:HD13	1.92	0.52
1:A:307:ILE:O	1:A:310:ILE:HG12	2.09	0.52
1:A:47:VAL:O	1:A:47:VAL:HG22	2.09	0.52
1:D:248:VAL:HG12	1:D:249:PRO:HD3	1.92	0.52
1:A:61:TRP:CZ2	1:A:138:MET:HE1	2.44	0.52
1:B:229:ARG:NH1	1:B:259:ILE:HG23	2.25	0.52
1:B:200:LEU:CD2	1:C:209:GLN:HG3	2.39	0.52
1:B:182:PHE:CA	1:B:185:LEU:HD12	2.32	0.52
1:D:304:LEU:HD23	1:D:307:ILE:HD11	1.91	0.52
1:D:240:PRO:HB2	1:D:241:PRO:HD3	1.91	0.52
1:A:232:LEU:HD13	1:A:254:VAL:HG12	1.91	0.51
1:C:99:VAL:HG21	1:C:235:LEU:CD1	2.40	0.51
1:B:77:GLY:HA3	1:B:87:LEU:HD21	1.92	0.51
1:E:77:GLY:HA3	1:E:87:LEU:HD21	1.90	0.51
1:E:78:GLU:O	1:E:81:GLY:N	2.40	0.51
1:C:302:MET:HB2	1:C:303:PRO:CD	2.40	0.51
1:E:117:LYS:O	1:E:118:ASN:HB3	2.10	0.51
1:A:26:ASP:O	1:A:68:HIS:NE2	2.36	0.51
1:D:197:GLU:O	1:D:200:LEU:HD12	2.10	0.51
1:A:242:LEU:HD22	1:A:251:PHE:CE1	2.45	0.51
1:D:244:GLU:O	1:D:246:GLU:N	2.43	0.51
1:B:200:LEU:HD22	1:C:209:GLN:HG3	1.93	0.51
1:B:311:TYR:HE2	1:B:330:VAL:HG21	1.74	0.51
1:A:77:GLY:HA3	1:A:87:LEU:CD1	2.40	0.51
1:E:182:PHE:HA	1:E:185:LEU:HD12	1.91	0.51
1:A:299:THR:HG21	1:A:345:PHE:CE1	2.46	0.51
1:D:119:LEU:HD12	1:D:119:LEU:O	2.11	0.51
1:C:201:GLU:C	1:C:203:PRO:HD3	2.31	0.51
1:B:222:ALA:CB	1:B:265:VAL:HG11	2.40	0.51
1:B:299:THR:HG21	1:B:345:PHE:CZ	2.46	0.51
1:B:51:LEU:HD22	1:B:79:PHE:CG	2.45	0.51
1:D:331:LEU:CD2	1:D:334:MET:HE2	2.41	0.51
1:C:242:LEU:HD22	1:C:251:PHE:CE1	2.46	0.51
1:D:272:VAL:O	1:D:275:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:HG21	1:C:345:PHE:HZ	1.72	0.50
1:C:28:GLU:OE2	1:C:143:ILE:HD11	2.11	0.50
1:B:238:ASP:O	1:B:239:VAL:O	2.29	0.50
1:A:294:LEU:HD21	1:B:294:LEU:HD11	1.92	0.50
1:D:66:GLY:N	1:D:140:GLN:O	2.44	0.50
1:B:299:THR:HG23	1:B:300:ILE:HG23	1.92	0.50
1:A:298:ALA:HA	1:E:302:MET:CE	2.42	0.50
1:A:61:TRP:HB2	1:A:169:LEU:CD2	2.41	0.50
1:B:171:TYR:CD2	1:B:172:SER:N	2.79	0.50
1:D:291:MET:CE	1:E:291:MET:HG2	2.40	0.50
1:A:101:PHE:CD1	1:A:106:VAL:HG13	2.47	0.50
1:A:82:ILE:HD13	1:A:130:ILE:CD1	2.41	0.50
1:A:229:ARG:HG3	1:A:258:THR:HG23	1.92	0.50
1:C:313:MET:CE	1:D:308:ALA:HB1	2.40	0.50
1:A:47:VAL:CB	1:A:72:VAL:HG13	2.41	0.50
1:E:272:VAL:HG13	1:E:275:LEU:HD22	1.94	0.50
1:C:116:ASP:OD2	1:C:119:LEU:HB3	2.11	0.50
1:E:221:LEU:O	1:E:222:ALA:C	2.50	0.50
1:B:221:LEU:O	1:B:225:ILE:HD12	2.11	0.50
1:C:184:LEU:O	1:C:188:ILE:HD12	2.11	0.50
1:D:336:VAL:O	1:D:340:ILE:HG23	2.12	0.50
1:D:299:THR:HG21	1:D:345:PHE:HZ	1.76	0.50
1:A:202:ARG:N	1:A:203:PRO:HD3	2.27	0.50
1:A:84:PRO:O	1:A:87:LEU:N	2.45	0.50
1:E:147:PHE:O	1:E:148:ASP:C	2.50	0.50
1:C:327:TYR:CZ	1:C:331:LEU:HD11	2.47	0.50
1:C:87:LEU:HA	1:C:90:ILE:HD12	1.94	0.50
1:E:109:VAL:CG1	1:E:126:GLN:OE1	2.59	0.49
1:C:250:TYR:O	1:C:253:ASP:HB3	2.12	0.49
1:E:177:LEU:HD21	1:E:181:TYR:HE1	1.77	0.49
1:B:313:MET:HE1	1:C:311:TYR:HB2	1.95	0.49
1:D:138:MET:C	1:D:139:PHE:CD2	2.85	0.49
1:A:91:LEU:O	1:A:93:VAL:HG13	2.13	0.49
1:B:112:MET:HE2	1:B:127:VAL:CG2	2.42	0.49
1:C:146:VAL:HG21	1:C:177:LEU:HA	1.94	0.49
1:D:36:ILE:CD1	1:D:163:LYS:CG	2.90	0.49
1:C:99:VAL:HG21	1:C:235:LEU:HD13	1.93	0.49
1:A:240:PRO:HB2	1:A:241:PRO:CD	2.42	0.49
1:A:228:LEU:O	1:A:231:VAL:HB	2.12	0.49
1:D:120:HIS:CE1	1:D:210:ARG:HG2	2.47	0.49
1:A:105:TYR:HB3	1:A:132:THR:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:CG2	1:A:300:ILE:HG23	2.43	0.49
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.94	0.49
1:B:164:LYS:HB3	1:B:168:TYR:CB	2.42	0.49
1:B:298:ALA:HB1	1:C:294:LEU:HD21	1.95	0.49
1:A:95:GLN:HA	1:E:260:GLN:HE22	1.78	0.49
1:A:171:TYR:CZ	1:A:250:TYR:HB3	2.48	0.49
1:A:165:ARG:NH1	1:A:243:ILE:HD13	2.27	0.49
1:B:222:ALA:HA	1:B:225:ILE:CD1	2.43	0.49
1:E:185:LEU:O	1:E:188:ILE:N	2.46	0.49
1:B:62:ILE:O	1:B:138:MET:N	2.40	0.49
1:D:214:LEU:O	1:D:215:LYS:C	2.50	0.49
1:D:56:SER:O	1:D:134:ASN:ND2	2.44	0.49
1:E:336:VAL:O	1:E:340:ILE:HG23	2.13	0.49
1:D:314:ASN:N	1:D:314:ASN:HD22	2.11	0.49
1:A:235:LEU:HD23	1:A:251:PHE:CD2	2.48	0.48
1:A:308:ALA:HB1	1:E:309:GLY:O	2.13	0.48
1:D:31:VAL:HG12	1:D:32:MET:N	2.28	0.48
1:B:90:ILE:O	1:B:90:ILE:HG22	2.12	0.48
1:B:257:HIS:O	1:B:260:GLN:HB3	2.13	0.48
1:A:302:MET:HG2	1:E:302:MET:HE1	1.95	0.48
1:C:219:VAL:HG22	1:C:269:ARG:HH11	1.77	0.48
1:D:167:ASP:OD1	1:D:168:TYR:N	2.46	0.48
1:B:82:ILE:CD1	1:B:130:ILE:HD13	2.42	0.48
1:A:291:MET:HE2	1:B:291:MET:HG2	1.96	0.48
1:D:99:VAL:HG23	1:D:231:VAL:CG1	2.34	0.48
1:A:175:ASP:OD1	1:A:254:VAL:HG22	2.13	0.48
1:B:242:LEU:HD22	1:B:251:PHE:HE1	1.75	0.48
1:C:343:VAL:O	1:C:343:VAL:HG12	2.13	0.48
1:A:129:LEU:HD23	1:A:138:MET:HA	1.96	0.48
1:C:310:ILE:HG22	1:D:308:ALA:CB	2.44	0.48
1:C:225:ILE:CD1	1:C:265:VAL:HG21	2.40	0.48
1:E:241:PRO:O	1:E:242:LEU:HG	2.14	0.48
1:A:209:GLN:O	1:A:212:HIS:N	2.46	0.48
1:A:306:PHE:O	1:A:310:ILE:HG23	2.13	0.48
1:A:232:LEU:HD23	1:A:235:LEU:CD2	2.35	0.48
1:B:180:ASP:O	1:B:183:VAL:HB	2.13	0.48
1:C:182:PHE:HA	1:C:185:LEU:HD12	1.95	0.48
1:E:69:ARG:O	1:E:73:VAL:HG23	2.13	0.48
1:D:165:ARG:HH11	1:D:243:ILE:HG21	1.77	0.48
1:D:178:VAL:HG11	1:D:257:HIS:HB2	1.96	0.48
1:C:299:THR:HG21	1:C:345:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:O	1:B:294:LEU:CD2	2.62	0.48
1:D:70:THR:HG22	1:D:91:LEU:HD22	1.94	0.48
1:E:197:GLU:O	1:E:198:GLU:C	2.52	0.48
1:A:232:LEU:CD2	1:A:235:LEU:HD22	2.35	0.48
1:A:297:ILE:HG21	1:E:299:THR:HA	1.96	0.48
1:D:331:LEU:HA	1:D:334:MET:HE2	1.96	0.48
1:A:51:LEU:HD21	1:A:76:VAL:HG22	1.95	0.48
1:D:36:ILE:CD1	1:D:163:LYS:HG3	2.43	0.48
1:B:167:ASP:O	1:B:168:TYR:C	2.51	0.48
1:E:99:VAL:CG2	1:E:231:VAL:HG12	2.41	0.48
1:E:306:PHE:CE2	1:E:310:ILE:HG21	2.49	0.48
1:E:306:PHE:CZ	1:E:310:ILE:HG21	2.49	0.48
1:C:242:LEU:HD22	1:C:251:PHE:HE1	1.79	0.48
1:A:347:LYS:O	1:A:348:LYS:CB	2.56	0.48
1:C:295:THR:CG2	1:D:293:VAL:CG1	2.92	0.48
1:A:239:VAL:CG1	1:A:248:VAL:HG22	2.36	0.48
1:B:225:ILE:HG21	1:B:262:ALA:HA	1.95	0.48
1:D:188:ILE:O	1:D:189:ASP:C	2.52	0.48
1:E:185:LEU:HD22	1:E:264:THR:HG21	1.95	0.48
1:A:291:MET:HE1	1:B:290:VAL:HG12	1.96	0.48
1:E:184:LEU:O	1:E:188:ILE:CD1	2.62	0.47
1:A:177:LEU:O	1:A:180:ASP:CB	2.60	0.47
1:D:36:ILE:HG23	1:D:37:GLU:N	2.29	0.47
1:B:33:ASN:ND2	1:B:59:PRO:O	2.47	0.47
1:A:204:GLU:HG2	1:A:205:LYS:H	1.79	0.47
1:D:44:THR:OG1	1:D:45:THR:N	2.47	0.47
1:B:311:TYR:CE2	1:B:330:VAL:HG21	2.48	0.47
1:C:185:LEU:HD11	1:C:261:ILE:HG23	1.95	0.47
1:A:274:GLY:O	1:A:277:ASP:N	2.46	0.47
1:D:177:LEU:O	1:D:177:LEU:HD23	2.13	0.47
1:E:181:TYR:O	1:E:184:LEU:HB3	2.14	0.47
1:D:36:ILE:HD11	1:D:163:LYS:HG2	1.95	0.47
1:D:116:ASP:OD1	1:D:117:LYS:O	2.32	0.47
1:D:47:VAL:CG2	1:D:51:LEU:HD21	2.39	0.47
1:B:247:THR:O	1:B:250:TYR:N	2.47	0.47
1:B:102:PHE:O	1:B:103:GLU:C	2.53	0.47
1:D:169:LEU:HD12	1:D:169:LEU:C	2.34	0.47
1:C:99:VAL:HG11	1:C:235:LEU:HD11	1.95	0.47
1:B:177:LEU:C	1:B:177:LEU:HD23	2.35	0.47
1:C:167:ASP:HB2	1:C:242:LEU:CD2	2.36	0.47
1:E:307:ILE:HA	1:E:310:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLY:HA3	1:C:215:LYS:HZ1	1.80	0.47
1:B:278:VAL:HG13	1:C:208:VAL:HG12	1.96	0.47
1:B:307:ILE:CD1	1:B:334:MET:HG2	2.37	0.47
1:A:332:ALA:O	1:A:336:VAL:HG23	2.15	0.47
1:D:242:LEU:O	1:D:244:GLU:N	2.46	0.47
1:E:51:LEU:HD21	1:E:76:VAL:HG22	1.97	0.47
1:D:232:LEU:HD13	1:D:258:THR:OG1	2.15	0.47
1:E:275:LEU:O	1:E:278:VAL:HB	2.14	0.47
1:D:332:ALA:O	1:D:336:VAL:HG23	2.14	0.47
1:C:288:ASN:O	1:C:291:MET:HB2	2.15	0.47
1:A:161:ILE:HD12	1:A:172:SER:OG	2.15	0.47
1:D:89:ASP:O	1:D:90:ILE:C	2.53	0.47
1:C:125:GLU:HG3	1:C:141:GLU:HB2	1.97	0.47
1:B:220:GLU:O	1:B:223:ALA:HB3	2.15	0.47
1:C:69:ARG:HB3	1:C:72:VAL:HG23	1.97	0.47
1:C:346:LYS:CE	1:C:349:LYS:HZ1	2.28	0.47
1:E:111:LYS:O	1:E:177:LEU:HD11	2.14	0.47
1:B:36:ILE:HG23	1:B:37:GLU:N	2.30	0.47
1:B:61:TRP:O	1:B:61:TRP:CD1	2.68	0.47
1:E:293:VAL:HG12	1:E:294:LEU:N	2.30	0.47
1:C:254:VAL:O	1:C:257:HIS:N	2.48	0.47
1:E:171:TYR:CE1	1:E:254:VAL:HG23	2.49	0.46
1:B:240:PRO:HG2	1:B:241:PRO:HD2	1.97	0.46
1:B:295:THR:HG21	1:C:293:VAL:HG12	1.96	0.46
1:E:244:GLU:O	1:E:246:GLU:N	2.48	0.46
1:E:206:GLU:O	1:E:209:GLN:HB2	2.14	0.46
1:E:99:VAL:HG22	1:E:231:VAL:CG1	2.43	0.46
1:A:299:THR:CG2	1:A:300:ILE:N	2.78	0.46
1:A:67:ILE:HD11	1:A:93:VAL:HG11	1.95	0.46
1:E:169:LEU:O	1:E:173:LEU:HD12	2.15	0.46
1:A:148:ASP:N	1:A:149:PRO:HD2	2.30	0.46
1:A:199:VAL:HG13	1:A:279:TYR:CA	2.45	0.46
1:C:51:LEU:N	1:C:52:PRO:HD2	2.30	0.46
1:A:298:ALA:O	1:A:299:THR:C	2.53	0.46
1:C:221:LEU:CD2	1:C:265:VAL:HG22	2.45	0.46
1:C:296:ILE:CD1	1:C:297:ILE:HD12	2.45	0.46
1:E:112:MET:SD	1:E:146:VAL:HG22	2.55	0.46
1:E:184:LEU:HD12	1:E:184:LEU:C	2.32	0.46
1:B:296:ILE:HD12	1:B:297:ILE:HD12	1.98	0.46
1:E:76:VAL:HG13	1:E:80:PHE:CE2	2.50	0.46
1:E:239:VAL:O	1:E:239:VAL:CG2	2.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLY:O	1:D:82:ILE:HB	2.15	0.46
1:C:200:LEU:HD22	1:D:209:GLN:CG	2.45	0.46
1:A:263:ASP:O	1:A:264:THR:C	2.54	0.46
1:E:304:LEU:HD23	1:E:307:ILE:CD1	2.26	0.46
1:D:86:VAL:O	1:D:89:ASP:HB2	2.15	0.46
1:A:312:GLY:HA2	1:E:312:GLY:O	2.16	0.46
1:A:47:VAL:CG2	1:A:76:VAL:HG23	2.46	0.46
1:D:247:THR:O	1:D:250:TYR:N	2.49	0.46
1:A:93:VAL:HB	1:A:141:GLU:OE2	2.15	0.46
1:A:59:PRO:HA	1:A:134:ASN:HB3	1.96	0.46
1:D:140:GLN:HE22	1:D:145:ASP:CB	2.28	0.46
1:D:44:THR:OG1	1:D:46:ASP:N	2.44	0.46
1:B:177:LEU:CD2	1:B:181:TYR:CE1	2.95	0.46
1:E:335:GLY:O	1:E:339:VAL:CG2	2.59	0.46
1:D:99:VAL:HG21	1:D:231:VAL:CG1	2.24	0.46
1:E:177:LEU:HD23	1:E:178:VAL:N	2.30	0.46
1:E:186:GLU:O	1:E:189:ASP:N	2.49	0.46
1:B:131:LEU:HD13	1:B:136:VAL:HG23	1.98	0.46
1:D:263:ASP:O	1:D:264:THR:C	2.54	0.46
1:E:211:THR:HG23	1:E:275:LEU:HD23	1.96	0.46
1:D:88:GLU:O	1:D:89:ASP:C	2.54	0.46
1:C:95:GLN:H	1:C:111:LYS:NZ	2.14	0.46
1:E:247:THR:HG22	1:E:251:PHE:CD1	2.50	0.46
1:B:296:ILE:HD12	1:B:297:ILE:N	2.30	0.46
1:D:31:VAL:HG21	1:D:50:VAL:HG12	1.97	0.46
1:E:56:SER:O	1:E:134:ASN:ND2	2.42	0.46
1:B:274:GLY:CA	1:C:215:LYS:HZ1	2.28	0.46
1:B:279:TYR:O	1:B:283:VAL:HG23	2.15	0.46
1:D:63:ASN:C	1:D:63:ASN:OD1	2.55	0.46
1:A:231:VAL:HG12	1:A:232:LEU:N	2.30	0.45
1:D:297:ILE:HG22	1:D:298:ALA:H	1.79	0.45
1:B:106:VAL:HG12	1:B:107:PHE:N	2.31	0.45
1:E:61:TRP:CZ2	1:E:173:LEU:HD21	2.51	0.45
1:C:30:GLU:HB3	1:C:63:ASN:HB3	1.99	0.45
1:C:179:ASP:O	1:C:182:PHE:HB2	2.16	0.45
1:A:306:PHE:CZ	1:A:310:ILE:HG21	2.51	0.45
1:D:88:GLU:O	1:D:91:LEU:N	2.49	0.45
1:C:199:VAL:HG13	1:C:279:TYR:CA	2.46	0.45
1:B:292:LYS:NZ	1:B:349:LYS:C	2.69	0.45
1:B:46:ASP:OD1	1:B:46:ASP:C	2.54	0.45
1:B:238:ASP:O	1:B:239:VAL:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:HD21	1:C:272:VAL:HG21	1.98	0.45
1:C:313:MET:N	1:C:313:MET:HE2	2.32	0.45
1:A:196:GLU:OE1	1:B:216:ARG:HD2	2.17	0.45
1:C:345:PHE:O	1:C:349:LYS:HB3	2.16	0.45
1:D:77:GLY:HA3	1:D:87:LEU:CD2	2.47	0.45
1:C:140:GLN:OE1	1:C:145:ASP:HB3	2.17	0.45
1:C:302:MET:HE2	1:D:298:ALA:HA	1.99	0.45
1:A:63:ASN:HA	1:A:138:MET:HB3	1.99	0.45
1:D:227:PRO:O	1:D:230:GLU:N	2.50	0.45
1:A:230:GLU:OE1	1:A:230:GLU:HA	2.16	0.45
1:D:167:ASP:OD2	1:D:243:ILE:HG12	2.17	0.45
1:E:189:ASP:O	1:E:192:ILE:HB	2.15	0.45
1:B:195:LEU:HD13	1:B:210:ARG:CZ	2.46	0.45
1:A:291:MET:HE3	1:B:290:VAL:HB	1.99	0.45
1:A:311:TYR:HB2	1:E:313:MET:HE1	1.97	0.45
1:A:277:ASP:OD1	1:A:277:ASP:N	2.49	0.45
1:E:243:ILE:HD12	1:E:246:GLU:HB3	1.99	0.45
1:D:82:ILE:CG2	1:D:87:LEU:HG	2.46	0.45
1:E:96:ARG:HD2	1:E:227:PRO:HB3	1.99	0.45
1:A:339:VAL:HA	1:A:342:VAL:CG2	2.46	0.45
1:E:93:VAL:HG11	1:E:141:GLU:OE1	2.17	0.45
1:C:60:THR:HG22	1:C:61:TRP:N	2.31	0.45
1:B:292:LYS:HZ2	1:B:349:LYS:HA	1.81	0.45
1:B:191:GLU:HB3	1:B:214:LEU:HD11	1.99	0.45
1:D:296:ILE:HG22	1:D:345:PHE:CE1	2.51	0.45
1:A:216:ARG:O	1:A:219:VAL:N	2.50	0.45
1:B:91:LEU:O	1:B:93:VAL:HG13	2.17	0.45
1:E:77:GLY:HA2	1:E:87:LEU:HD21	1.98	0.45
1:B:199:VAL:HG13	1:B:279:TYR:HB2	1.97	0.45
1:E:118:ASN:O	1:E:120:HIS:N	2.50	0.45
1:E:225:ILE:HD13	1:E:261:ILE:HG22	1.98	0.45
1:C:26:ASP:O	1:C:68:HIS:NE2	2.41	0.45
1:B:101:PHE:CZ	1:B:235:LEU:HD12	2.52	0.45
1:D:189:ASP:O	1:D:192:ILE:HB	2.17	0.45
1:D:132:THR:O	1:D:134:ASN:N	2.50	0.45
1:A:264:THR:O	1:A:267:THR:CB	2.65	0.45
1:A:239:VAL:HG12	1:A:242:LEU:HD12	1.99	0.44
1:B:242:LEU:HD21	1:B:251:PHE:HE1	1.60	0.44
1:D:306:PHE:HB2	1:E:305:THR:OG1	2.17	0.44
1:C:261:ILE:O	1:C:262:ALA:C	2.55	0.44
1:D:331:LEU:HA	1:D:334:MET:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:TYR:OH	1:B:120:HIS:HA	2.17	0.44
1:D:302:MET:HE1	1:E:298:ALA:HA	1.99	0.44
1:A:200:LEU:HD13	1:B:209:GLN:HE21	1.82	0.44
1:E:51:LEU:N	1:E:52:PRO:HD2	2.33	0.44
1:A:99:VAL:HG13	1:A:108:ILE:HG12	1.98	0.44
1:A:47:VAL:CG2	1:A:72:VAL:CG1	2.89	0.44
1:E:146:VAL:HG21	1:E:177:LEU:HA	2.00	0.44
1:A:331:LEU:HD23	1:A:334:MET:HE2	1.98	0.44
1:B:200:LEU:HD21	1:C:209:GLN:HG2	2.00	0.44
1:E:247:THR:HG22	1:E:251:PHE:CE1	2.53	0.44
1:D:178:VAL:HG21	1:D:254:VAL:HG13	1.98	0.44
1:E:182:PHE:O	1:E:183:VAL:C	2.54	0.44
1:E:332:ALA:O	1:E:336:VAL:N	2.48	0.44
1:A:51:LEU:N	1:A:52:PRO:HD2	2.32	0.44
1:D:291:MET:HB3	1:D:291:MET:HE3	1.86	0.44
1:C:302:MET:HE3	1:C:302:MET:HB3	1.78	0.44
1:D:247:THR:O	1:D:248:VAL:C	2.56	0.44
1:A:90:ILE:HD13	1:A:139:PHE:CE1	2.52	0.44
1:A:339:VAL:O	1:A:343:VAL:HG23	2.17	0.44
1:D:296:ILE:C	1:D:296:ILE:HD12	2.38	0.44
1:D:147:PHE:O	1:D:151:ARG:HG3	2.18	0.44
1:B:177:LEU:O	1:B:180:ASP:N	2.50	0.44
1:D:313:MET:SD	1:E:311:TYR:HB2	2.58	0.44
1:B:240:PRO:HB2	1:B:241:PRO:HD2	1.95	0.44
1:D:168:TYR:O	1:D:169:LEU:C	2.52	0.44
1:A:268:PHE:O	1:A:269:ARG:C	2.56	0.44
1:E:213:GLN:O	1:E:214:LEU:C	2.54	0.44
1:C:219:VAL:HG22	1:C:269:ARG:NH1	2.32	0.43
1:B:244:GLU:O	1:B:245:LYS:C	2.56	0.43
1:B:165:ARG:O	1:B:166:ALA:C	2.56	0.43
1:C:148:ASP:N	1:C:149:PRO:CD	2.81	0.43
1:C:127:VAL:HG22	1:C:140:GLN:HG2	2.01	0.43
1:C:140:GLN:HE22	1:C:145:ASP:CB	2.30	0.43
1:A:73:VAL:O	1:A:87:LEU:HD22	2.18	0.43
1:E:208:VAL:O	1:E:209:GLN:C	2.55	0.43
1:B:197:GLU:HA	1:B:197:GLU:OE1	2.19	0.43
1:D:225:ILE:CD1	1:D:265:VAL:HG21	2.47	0.43
1:E:63:ASN:HB2	1:E:138:MET:HE2	2.00	0.43
1:A:200:LEU:HD13	1:A:201:GLU:HG3	2.00	0.43
1:E:92:ASN:O	1:E:95:GLN:NE2	2.52	0.43
1:E:167:ASP:O	1:E:170:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:MET:HA	1:A:313:MET:CE	2.49	0.43
1:E:64:ILE:HD12	1:E:138:MET:O	2.18	0.43
1:D:171:TYR:CD2	1:D:172:SER:N	2.86	0.43
1:D:173:LEU:O	1:D:176:ALA:HB3	2.18	0.43
1:A:64:ILE:N	1:A:138:MET:O	2.43	0.43
1:A:221:LEU:C	1:A:225:ILE:HD12	2.37	0.43
1:D:89:ASP:OD1	1:D:95:GLN:OE1	2.37	0.43
1:A:171:TYR:HE1	1:A:254:VAL:HG23	1.83	0.43
1:C:130:ILE:CG2	1:C:137:LEU:HD12	2.48	0.43
1:A:177:LEU:C	1:A:177:LEU:HD23	2.38	0.43
1:B:129:LEU:HD23	1:B:138:MET:HA	2.00	0.43
1:D:243:ILE:O	1:D:244:GLU:O	2.37	0.43
1:B:86:VAL:HG13	1:B:107:PHE:CZ	2.54	0.43
1:E:227:PRO:O	1:E:228:LEU:C	2.57	0.43
1:C:302:MET:HE2	1:D:297:ILE:C	2.39	0.43
1:E:177:LEU:HD23	1:E:177:LEU:O	2.18	0.43
1:A:99:VAL:HG22	1:A:231:VAL:HG22	2.01	0.43
1:D:264:THR:O	1:D:267:THR:HB	2.18	0.43
1:D:272:VAL:O	1:D:273:SER:C	2.57	0.43
1:D:148:ASP:O	1:D:152:GLU:HG2	2.19	0.43
1:C:86:VAL:O	1:C:89:ASP:HB2	2.19	0.43
1:C:83:HIS:HD1	1:C:84:PRO:HD2	1.84	0.43
1:B:115:TYR:CZ	1:B:120:HIS:HA	2.54	0.43
1:B:310:ILE:HG22	1:C:308:ALA:HB2	2.01	0.42
1:C:296:ILE:HD11	1:C:297:ILE:HD12	2.01	0.42
1:B:218:LEU:HD21	1:B:268:PHE:HB3	1.99	0.42
1:E:302:MET:N	1:E:303:PRO:HD2	2.35	0.42
1:B:221:LEU:C	1:B:225:ILE:HD12	2.40	0.42
1:C:243:ILE:HD12	1:C:246:GLU:HB3	1.99	0.42
1:D:172:SER:O	1:D:173:LEU:C	2.57	0.42
1:C:296:ILE:C	1:C:296:ILE:HD12	2.39	0.42
1:D:128:SER:HB2	1:D:139:PHE:HB2	2.00	0.42
1:C:128:SER:O	1:C:129:LEU:HD23	2.19	0.42
1:A:216:ARG:NH1	1:E:196:GLU:OE1	2.52	0.42
1:E:179:ASP:O	1:E:181:TYR:N	2.53	0.42
1:D:229:ARG:HG3	1:D:258:THR:HG22	2.00	0.42
1:B:84:PRO:O	1:B:85:LEU:C	2.58	0.42
1:B:64:ILE:CD1	1:B:76:VAL:HG21	2.50	0.42
1:A:299:THR:HG23	1:A:300:ILE:N	2.34	0.42
1:E:296:ILE:O	1:E:300:ILE:HG23	2.19	0.42
1:E:199:VAL:HG13	1:E:279:TYR:CB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ARG:N	1:C:203:PRO:HD3	2.34	0.42
1:C:199:VAL:HG13	1:C:279:TYR:HA	2.01	0.42
1:C:265:VAL:HG12	1:C:269:ARG:HG3	2.02	0.42
1:E:140:GLN:HE22	1:E:145:ASP:HB3	1.84	0.42
1:B:46:ASP:OD2	1:B:49:SER:HB3	2.19	0.42
1:B:64:ILE:HD11	1:B:76:VAL:HG21	2.01	0.42
1:D:297:ILE:O	1:D:298:ALA:C	2.58	0.42
1:B:177:LEU:O	1:B:178:VAL:C	2.56	0.42
1:E:200:LEU:HD12	1:E:201:GLU:HG2	2.02	0.42
1:D:36:ILE:HD13	1:D:163:LYS:HA	2.02	0.42
1:E:206:GLU:O	1:E:207:THR:C	2.56	0.42
1:C:122:LEU:HD22	1:C:217:ASN:ND2	2.34	0.42
1:A:297:ILE:HG22	1:A:298:ALA:N	2.35	0.42
1:E:306:PHE:CD1	1:E:307:ILE:HG23	2.53	0.42
1:B:171:TYR:C	1:B:171:TYR:CD2	2.92	0.42
1:C:99:VAL:HG11	1:C:235:LEU:CD1	2.50	0.42
1:D:77:GLY:CA	1:D:87:LEU:HD21	2.50	0.42
1:B:200:LEU:HD21	1:C:209:GLN:CG	2.50	0.42
1:D:302:MET:HE1	1:E:302:MET:HG2	2.02	0.42
1:B:225:ILE:O	1:B:228:LEU:HB3	2.20	0.42
1:C:295:THR:O	1:C:299:THR:HB	2.19	0.42
1:E:185:LEU:HD22	1:E:264:THR:CG2	2.49	0.42
1:A:62:ILE:HD12	1:A:137:LEU:CD2	2.50	0.42
1:A:106:VAL:HG12	1:A:107:PHE:N	2.35	0.42
1:A:181:TYR:O	1:A:184:LEU:HB3	2.20	0.42
1:E:129:LEU:HD23	1:E:138:MET:HA	2.02	0.42
1:A:331:LEU:HD23	1:A:334:MET:HE1	2.02	0.42
1:A:44:THR:HG21	1:A:49:SER:OG	2.20	0.42
1:E:129:LEU:HA	1:E:137:LEU:O	2.20	0.42
1:D:122:LEU:CD2	1:D:217:ASN:ND2	2.70	0.42
1:D:171:TYR:CG	1:D:172:SER:N	2.87	0.42
1:B:295:THR:HA	1:C:294:LEU:HG	2.02	0.42
1:B:218:LEU:HD21	1:B:268:PHE:CB	2.50	0.42
1:B:110:LEU:HD22	1:B:228:LEU:CD1	2.49	0.41
1:E:240:PRO:CB	1:E:241:PRO:CD	2.97	0.41
1:A:292:LYS:O	1:A:293:VAL:C	2.57	0.41
1:B:202:ARG:N	1:B:203:PRO:HD3	2.35	0.41
1:C:112:MET:SD	1:C:146:VAL:HG13	2.60	0.41
1:A:266:GLU:O	1:A:267:THR:C	2.58	0.41
1:C:268:PHE:O	1:C:269:ARG:C	2.58	0.41
1:D:177:LEU:C	1:D:177:LEU:CD2	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LEU:O	1:D:178:VAL:C	2.57	0.41
1:B:61:TRP:O	1:B:61:TRP:CG	2.73	0.41
1:D:36:ILE:HD11	1:D:163:LYS:CG	2.49	0.41
1:A:308:ALA:HB2	1:E:310:ILE:HG22	2.03	0.41
1:E:296:ILE:HG22	1:E:345:PHE:CZ	2.53	0.41
1:D:239:VAL:HA	1:D:242:LEU:HD12	2.02	0.41
1:C:310:ILE:O	1:C:313:MET:HE2	2.20	0.41
1:B:112:MET:HE1	1:B:127:VAL:HG21	2.03	0.41
1:C:298:ALA:O	1:C:302:MET:CG	2.68	0.41
1:E:171:TYR:O	1:E:174:ILE:HB	2.20	0.41
1:B:330:VAL:O	1:B:334:MET:HG3	2.21	0.41
1:B:221:LEU:HG	1:B:225:ILE:HD11	2.02	0.41
1:B:70:THR:HG22	1:B:91:LEU:CD2	2.45	0.41
1:B:295:THR:CG2	1:C:293:VAL:HG12	2.49	0.41
1:E:34:TYR:OH	1:E:169:LEU:HD22	2.20	0.41
1:B:164:LYS:HB3	1:B:168:TYR:HB3	2.02	0.41
1:A:280:LEU:HA	1:A:280:LEU:HD12	1.92	0.41
1:D:97:PRO:HG3	1:D:111:LYS:HG2	2.02	0.41
1:A:47:VAL:HG22	1:A:76:VAL:HG23	2.02	0.41
1:D:129:LEU:O	1:D:130:ILE:HG13	2.21	0.41
1:B:84:PRO:HA	1:B:87:LEU:HD12	2.03	0.41
1:B:86:VAL:O	1:B:87:LEU:C	2.59	0.41
1:E:235:LEU:HD23	1:E:251:PHE:CE2	2.56	0.41
1:A:77:GLY:CA	1:A:87:LEU:HD11	2.50	0.41
1:D:240:PRO:CB	1:D:241:PRO:CD	2.99	0.41
1:A:280:LEU:HD21	1:E:280:LEU:HD23	2.01	0.41
1:E:232:LEU:HD13	1:E:258:THR:HB	2.03	0.41
1:A:221:LEU:CD1	1:A:225:ILE:HD11	2.50	0.41
1:C:277:ASP:N	1:C:277:ASP:OD1	2.54	0.41
1:A:51:LEU:CD2	1:A:76:VAL:HG22	2.51	0.41
1:B:292:LYS:HZ1	1:B:349:LYS:C	2.23	0.41
1:E:175:ASP:O	1:E:176:ALA:C	2.59	0.41
1:C:302:MET:HE2	1:D:298:ALA:N	2.35	0.41
1:C:221:LEU:HD23	1:C:265:VAL:CG2	2.47	0.41
1:E:256:ASP:CA	1:E:259:ILE:HD12	2.49	0.41
1:C:117:LYS:O	1:C:119:LEU:N	2.53	0.41
1:B:304:LEU:HD11	1:B:338:ALA:HB2	2.03	0.41
1:C:302:MET:HB2	1:C:303:PRO:HD3	2.02	0.41
1:A:65:THR:HG21	1:A:143:ILE:CG1	2.50	0.41
1:E:125:GLU:HG3	1:E:141:GLU:HB2	2.03	0.41
1:D:329:VAL:HA	1:D:332:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:GLU:O	1:E:209:GLN:N	2.54	0.41
1:C:38:GLU:HG2	1:C:39:PHE:N	2.36	0.41
1:D:296:ILE:C	1:D:299:THR:HG22	2.42	0.40
1:D:243:ILE:HD12	1:D:246:GLU:CB	2.47	0.40
1:D:275:LEU:O	1:D:276:LEU:C	2.59	0.40
1:E:53:PHE:O	1:E:54:ARG:C	2.60	0.40
1:C:337:ILE:O	1:C:341:MET:HG2	2.21	0.40
1:E:127:VAL:HA	1:E:139:PHE:O	2.21	0.40
1:B:177:LEU:HD23	1:B:178:VAL:N	2.37	0.40
1:D:171:TYR:HE1	1:D:254:VAL:CG2	2.35	0.40
1:B:297:ILE:O	1:B:298:ALA:C	2.59	0.40
1:D:327:TYR:N	1:D:328:PRO:HD2	2.36	0.40
1:C:195:LEU:C	1:C:197:GLU:H	2.23	0.40
1:B:65:THR:CG2	1:B:143:ILE:HD13	2.49	0.40
1:D:195:LEU:HD21	1:D:211:THR:CA	2.50	0.40
1:E:224:THR:O	1:E:228:LEU:HB2	2.21	0.40
1:E:225:ILE:HD13	1:E:261:ILE:CG2	2.52	0.40
1:E:341:MET:O	1:E:344:TYR:HB3	2.22	0.40
1:D:26:ASP:O	1:D:68:HIS:NE2	2.44	0.40
1:A:242:LEU:O	1:A:243:ILE:C	2.59	0.40
1:D:299:THR:HG21	1:D:345:PHE:CE1	2.56	0.40
1:A:337:ILE:HA	1:A:340:ILE:HG12	2.04	0.40
1:E:177:LEU:HD21	1:E:181:TYR:CE1	2.57	0.40
1:A:330:VAL:HG12	1:A:334:MET:HG3	2.02	0.40
1:D:259:ILE:O	1:D:260:GLN:C	2.60	0.40
1:D:337:ILE:HA	1:D:340:ILE:HG12	2.03	0.40
1:A:278:VAL:HA	1:B:276:LEU:HD21	2.02	0.40
1:E:274:GLY:O	1:E:277:ASP:HB2	2.21	0.40
1:D:225:ILE:HD12	1:D:265:VAL:HG21	2.04	0.40
1:E:127:VAL:HG22	1:E:140:GLN:HG2	2.03	0.40
1:B:101:PHE:CD1	1:B:240:PRO:HG3	2.57	0.40
1:E:178:VAL:O	1:E:181:TYR:HB2	2.22	0.40
1:A:330:VAL:O	1:A:334:MET:HG3	2.21	0.40
1:D:223:ALA:O	1:D:227:PRO:CD	2.69	0.40
1:E:132:THR:O	1:E:134:ASN:N	2.54	0.40
1:A:29:ILE:HB	1:A:44:THR:O	2.21	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	310/330 (94%)	255 (82%)	47 (15%)	8 (3%)	7	48
1	B	312/330 (94%)	251 (80%)	50 (16%)	11 (4%)	4	42
1	C	310/330 (94%)	255 (82%)	48 (16%)	7 (2%)	8	51
1	D	310/330 (94%)	246 (79%)	52 (17%)	12 (4%)	4	38
1	E	310/330 (94%)	250 (81%)	41 (13%)	19 (6%)	2	27
All	All	1552/1650 (94%)	1257 (81%)	238 (15%)	57 (4%)	4	40

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	240	PRO
1	A	348	LYS
1	B	240	PRO
1	B	246	GLU
1	B	348	LYS
1	C	240	PRO
1	D	240	PRO
1	D	244	GLU
1	E	240	PRO
1	E	243	ILE
1	A	244	GLU
1	A	275	LEU
1	A	293	VAL
1	B	103	GLU
1	B	157	ASN
1	B	239	VAL
1	C	238	ASP
1	C	239	VAL
1	C	244	GLU
1	D	243	ILE

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Mol	Chain	Res	Type
1	D	246	GLU
1	E	71	ASP
1	E	180	ASP
1	E	208	VAL
1	E	244	GLU
1	E	246	GLU
1	E	348	LYS
1	A	118	ASN
1	B	120	HIS
1	D	66	GLY
1	D	133	LYS
1	E	209	GLN
1	E	238	ASP
1	E	293	VAL
1	B	238	ASP
1	C	118	ASN
1	C	267	THR
1	D	59	PRO
1	E	118	ASN
1	A	239	VAL
1	B	243	ILE
1	D	239	VAL
1	D	245	LYS
1	D	258	THR
1	E	133	LYS
1	E	176	ALA
1	B	166	ALA
1	D	348	LYS
1	B	77	GLY
1	C	159	GLY
1	E	148	ASP
1	D	36	ILE
1	E	67	ILE
1	E	183	VAL
1	E	239	VAL
1	E	241	PRO

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	295/310 (95%)	273 (92%)	22 (8%)	17	57
1	B	295/310 (95%)	270 (92%)	25 (8%)	13	52
1	C	295/310 (95%)	272 (92%)	23 (8%)	16	55
1	D	295/310 (95%)	270 (92%)	25 (8%)	13	52
1	E	295/310 (95%)	278 (94%)	17 (6%)	25	66
All	All	1475/1550 (95%)	1363 (92%)	112 (8%)	16	56

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	40	ARG
1	A	44	THR
1	A	95	GLN
1	A	99	VAL
1	A	145	ASP
1	A	163	LYS
1	A	200	LEU
1	A	202	ARG
1	A	206	GLU
1	A	233	SER
1	A	238	ASP
1	A	258	THR
1	A	264	THR
1	A	277	ASP
1	A	281	SER
1	A	285	ASN
1	A	297	ILE
1	A	315	PHE
1	A	337	ILE
1	A	346	LYS
1	A	349	LYS
1	B	26	ASP
1	B	40	ARG
1	B	41	GLU
1	B	122	LEU
1	B	123	GLU
1	B	128	SER

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Mol	Chain	Res	Type
1	B	132	THR
1	B	164	LYS
1	B	165	ARG
1	B	171	TYR
1	B	198	GLU
1	B	206	GLU
1	B	218	LEU
1	B	233	SER
1	B	235	LEU
1	B	238	ASP
1	B	242	LEU
1	B	248	VAL
1	B	260	GLN
1	B	263	ASP
1	B	284	SER
1	B	294	LEU
1	B	327	TYR
1	B	337	ILE
1	B	346	LYS
1	C	38	GLU
1	C	40	ARG
1	C	93	VAL
1	C	95	GLN
1	C	96	ARG
1	C	123	GLU
1	C	165	ARG
1	C	172	SER
1	C	177	LEU
1	C	178	VAL
1	C	200	LEU
1	C	206	GLU
1	C	237	ARG
1	C	238	ASP
1	C	263	ASP
1	C	277	ASP
1	C	284	SER
1	C	294	LEU
1	C	297	ILE
1	C	307	ILE
1	C	346	LYS
1	C	347	LYS
1	C	349	LYS

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Mol	Chain	Res	Type
1	D	26	ASP
1	D	40	ARG
1	D	44	THR
1	D	85	LEU
1	D	95	GLN
1	D	96	ARG
1	D	119	LEU
1	D	122	LEU
1	D	143	ILE
1	D	152	GLU
1	D	165	ARG
1	D	169	LEU
1	D	206	GLU
1	D	226	TRP
1	D	232	LEU
1	D	238	ASP
1	D	248	VAL
1	D	267	THR
1	D	269	ARG
1	D	279	TYR
1	D	297	ILE
1	D	307	ILE
1	D	314	ASN
1	D	346	LYS
1	D	349	LYS
1	E	26	ASP
1	E	28	GLU
1	E	29	ILE
1	E	40	ARG
1	E	44	THR
1	E	65	THR
1	E	95	GLN
1	E	118	ASN
1	E	121	GLU
1	E	123	GLU
1	E	128	SER
1	E	184	LEU
1	E	211	THR
1	E	238	ASP
1	E	287	THR
1	E	297	ILE
1	E	346	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	213	GLN
1	A	217	ASN
1	A	285	ASN
1	B	33	ASN
1	B	120	HIS
1	B	140	GLN
1	B	209	GLN
1	B	257	HIS
1	B	314	ASN
1	C	33	ASN
1	C	95	GLN
1	C	118	ASN
1	C	140	GLN
1	C	217	ASN
1	C	314	ASN
1	D	33	ASN
1	D	140	GLN
1	D	217	ASN
1	D	260	GLN
1	D	314	ASN
1	E	33	ASN
1	E	120	HIS
1	E	140	GLN
1	E	217	ASN
1	E	288	ASN
1	E	314	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.24	6 (1%) 70 54	124, 172, 239, 320	0
1	B	316/330 (95%)	-0.56	2 (0%) 90 82	110, 148, 223, 326	0
1	C	314/330 (95%)	-0.56	2 (0%) 90 82	109, 142, 210, 320	0
1	D	314/330 (95%)	-0.58	1 (0%) 94 89	112, 144, 220, 327	0
1	E	314/330 (95%)	-0.42	3 (0%) 84 72	122, 157, 227, 329	0
All	All	1572/1650 (95%)	-0.47	14 (0%) 85 74	109, 152, 229, 329	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	LYS	4.7
1	C	315	PHE	3.5
1	A	38	GLU	3.4
1	B	314	ASN	3.3
1	C	326	GLY	3.0
1	B	326	GLY	3.0
1	A	36	ILE	2.7
1	A	68	HIS	2.6
1	A	35	SER	2.5
1	D	315	PHE	2.5
1	E	327	TYR	2.4
1	A	37	GLU	2.3
1	E	159	GLY	2.1
1	E	245	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CS	B	1001	1/1	0.73	0.21	1.43	170,170,170,170	1
2	CS	D	1001	1/1	0.64	0.22	0.85	158,158,158,158	1
2	CS	A	401	1/1	0.68	0.18	-2.64	281,281,281,281	1
2	CS	E	401	1/1	0.86	0.15	-	154,154,154,154	1
2	CS	B	1003	1/1	0.91	0.16	-	144,144,144,144	1
2	CS	E	402	1/1	0.89	0.21	-	155,155,155,155	1
2	CS	C	401	1/1	0.94	0.16	-	178,178,178,178	1
3	NA	B	1002	1/1	0.86	0.14	-	109,109,109,109	0
2	CS	B	1004	1/1	0.85	0.31	-	135,135,135,135	1
2	CS	E	403	1/1	0.94	0.22	-	183,183,183,183	1

6.5 Other polymers [i](#)

There are no such residues in this entry.