



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID : 3HAI
Title : Crystal structure of human PACSIN1 F-BAR domain (P21 lattice)
Authors : Wang, Q.; Navarro, M.V.A.S.; Peng, G.; Rajashankar, K.R.; Sondermann, H.
Deposited on : 2009-05-01
Resolution : 2.88 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

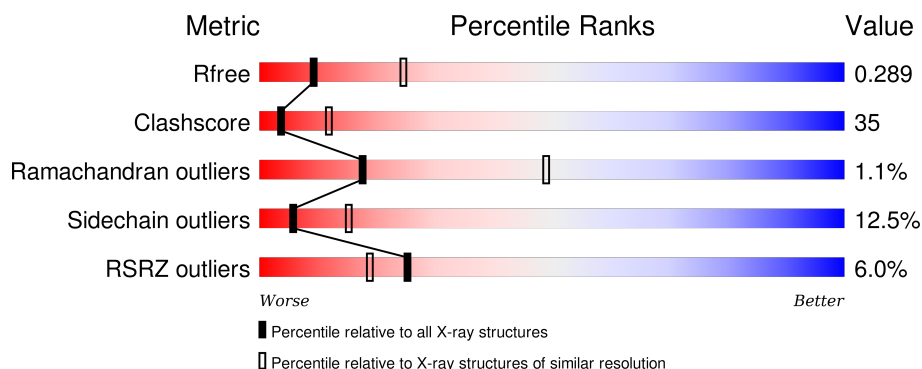
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	308	<div> <div>4%</div> <div>41% 43% 12% 5%</div> </div>
1	B	308	<div> <div>5%</div> <div>41% 48% 6% 5%</div> </div>
1	C	308	<div> <div>4%</div> <div>41% 46% 6% 7%</div> </div>
1	D	308	<div> <div>10%</div> <div>43% 38% 8% 10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	A	310	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9553 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 human PACSIN1 F-BAR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2441	1529	432	465	15			
1	B	294	Total	C	N	O	S	0	0	0
			2438	1527	432	464	15			
1	C	285	Total	C	N	O	S	0	0	0
			2359	1477	420	447	15			
1	D	276	Total	C	N	O	S	0	0	0
			2294	1441	408	430	15			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

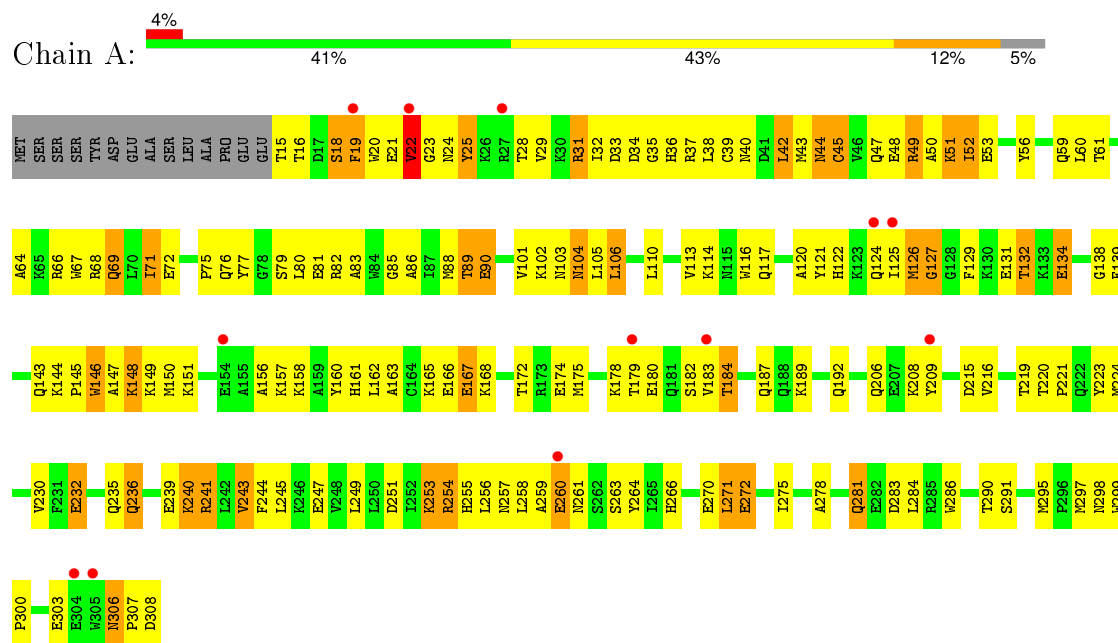
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	10	Total	O	0	0
			10	10		
3	C	2	Total	O	0	0
			2	2		
3	D	3	Total	O	0	0
			3	3		

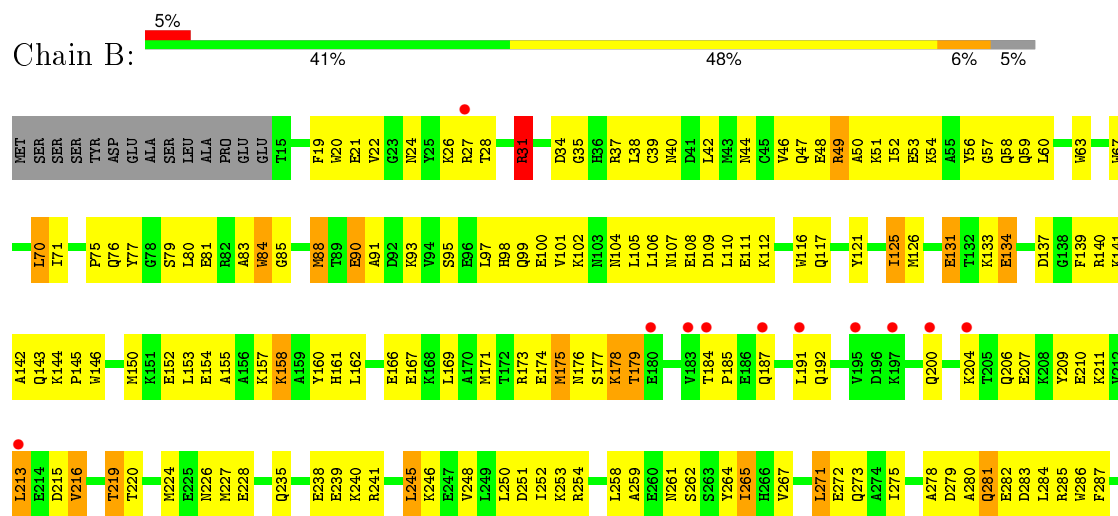
3 Residue-property plots

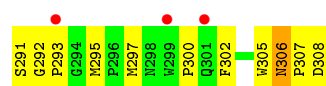
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: human PACSIN1 F-BAR

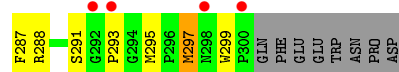
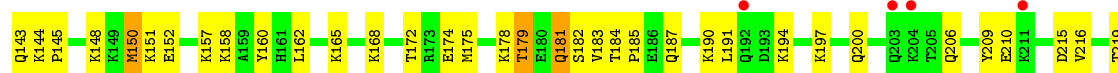
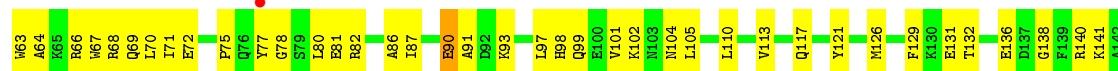
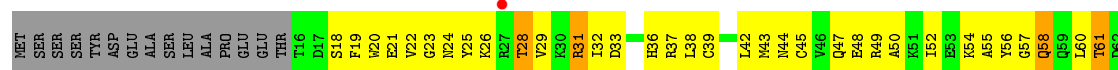


• Molecule 1: human PACSIN1 F-BAR

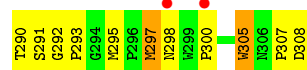
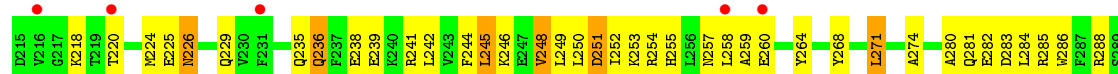
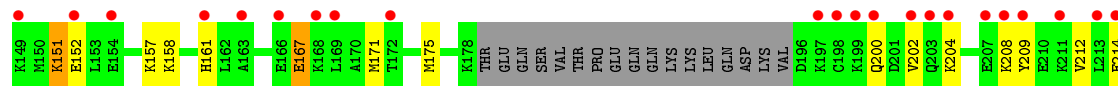
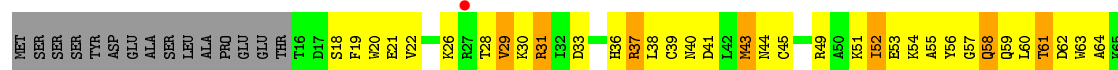
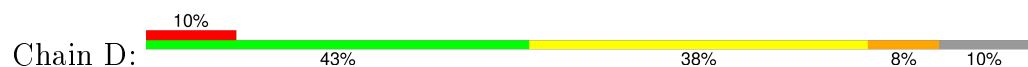




• Molecule 1: human PACSIN1 F-BAR



• Molecule 1: human PACSIN1 F-BAR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	163.62Å 32.16Å 181.16Å 90.00° 111.23° 90.00°	Depositor
Resolution (Å)	48.52 – 2.88 48.52 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.52-2.88) 97.9 (48.52-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 2009_02_15_2320_3)	Depositor
R, R_{free}	0.282 , 0.319 0.283 , 0.289	Depositor DCC
R_{free} test set	2052 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 40596 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9553	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% 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: CA

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	0.48	0/2489	0.63	0/3339
1	B	0.52	0/2486	0.60	0/3336
1	C	0.44	0/2403	0.56	0/3220
1	D	0.41	0/2340	0.55	0/3136
All	All	0.47	0/9718	0.59	0/13031

There are no bond length outliers.

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	2441	0	2395	237	0
1	B	2438	0	2388	196	0
1	C	2359	0	2332	186	0
1	D	2294	0	2241	184	0
2	A	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
All	All	9553	0	9356	669	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 35.

All (669) 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:A:241:ARG:HG3	1:A:241:ARG:HH21	1.17	1.08
1:D:130:LYS:HD3	1:D:131:GLU:H	1.13	1.08
1:D:140:ARG:HH11	1:D:140:ARG:HG2	1.21	1.05
1:C:297:MET:HG3	1:D:20:TRP:HB2	1.45	0.98
1:B:142:ALA:HB1	1:B:226:ASN:HB3	1.46	0.96
1:B:144:LYS:HB3	1:B:145:PRO:HD3	1.47	0.96
1:B:116:TRP:CH2	1:B:241:ARG:HB3	2.01	0.96
1:D:82:ARG:HH11	1:D:82:ARG:HG2	1.31	0.95
1:A:261:ASN:ND2	1:A:263:SER:HB2	1.81	0.94
1:D:130:LYS:HD3	1:D:131:GLU:N	1.82	0.94
1:B:90:GLU:HG3	1:B:91:ALA:N	1.82	0.93
1:A:183:VAL:HG13	1:A:184:THR:HG22	1.49	0.91
1:C:19:PHE:H	1:D:295:MET:HE2	1.34	0.91
1:A:257:ASN:ND2	1:A:260:GLU:HB2	1.85	0.91
1:A:272:GLU:HG3	1:B:253:LYS:HZ2	1.35	0.91
1:D:297:MET:HE3	1:D:297:MET:HA	1.55	0.88
1:C:206:GLN:O	1:C:210:GLU:HG3	1.74	0.88
1:C:56:TYR:HD1	1:D:56:TYR:HB2	1.40	0.86
1:B:116:TRP:HH2	1:B:241:ARG:HB3	1.39	0.85
1:A:249:LEU:O	1:B:275:ILE:HD13	1.76	0.85
1:B:31:ARG:HH22	1:B:235:GLN:HE21	1.21	0.85
1:C:58:GLN:HE21	1:C:58:GLN:HA	1.44	0.83
1:B:258:LEU:O	1:B:261:ASN:HB3	1.79	0.83
1:A:241:ARG:HH21	1:A:241:ARG:CG	1.91	0.82
1:C:36:HIS:O	1:C:39:CYS:HB2	1.80	0.81
1:B:143:GLN:HB2	1:B:227:MET:CE	2.10	0.81
1:D:82:ARG:HH11	1:D:82:ARG:CG	1.94	0.81
1:A:272:GLU:HG3	1:B:253:LYS:NZ	1.94	0.81
1:B:292:GLY:O	1:B:295:MET:HG2	1.80	0.80
1:A:19:PHE:HE1	1:B:293:PRO:HG3	1.46	0.80
1:A:241:ARG:HG3	1:A:241:ARG:NH2	1.89	0.80
1:C:250:LEU:HD12	1:C:254:ARG:HH12	1.46	0.80
1:A:182:SER:HB3	1:A:183:VAL:HB	1.63	0.79
1:A:261:ASN:HD21	1:A:263:SER:HB2	1.45	0.79
1:D:140:ARG:HH11	1:D:140:ARG:CG	1.94	0.79
1:A:183:VAL:HG22	1:A:184:THR:HA	1.63	0.79
1:A:69:GLN:HE21	1:A:69:GLN:HA	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:HB2	1:B:102:LYS:HD3	1.66	0.77
1:B:160:TYR:HE2	1:B:206:GLN:HB2	1.48	0.77
1:B:58:GLN:HA	1:B:58:GLN:NE2	2.00	0.77
1:A:264:TYR:CD2	1:B:259:ALA:HB2	2.20	0.77
1:A:28:THR:HG22	1:B:287:PHE:HE1	1.50	0.77
1:C:87:ILE:H	1:C:87:ILE:HD12	1.50	0.77
1:D:87:ILE:HD13	1:D:271:LEU:HD11	1.68	0.76
1:A:300:PRO:HG3	1:B:150:MET:HE3	1.67	0.76
1:A:44:ASN:N	1:A:44:ASN:HD22	1.84	0.76
1:A:264:TYR:HD2	1:B:259:ALA:HB2	1.51	0.75
1:A:81:GLU:HG3	1:A:82:ARG:N	2.01	0.75
1:A:182:SER:HB3	1:A:183:VAL:CB	2.17	0.75
1:C:258:LEU:HB2	1:D:264:TYR:OH	1.85	0.75
1:A:43:MET:CE	1:A:113:VAL:HG23	2.16	0.75
1:C:90:GLU:HG3	1:C:91:ALA:N	2.00	0.75
1:A:134:GLU:HG3	1:A:134:GLU:O	1.85	0.74
1:C:259:ALA:HB2	1:D:264:TYR:CD2	2.23	0.74
1:A:239:GLU:HB2	1:B:284:LEU:HD11	1.70	0.74
1:A:36:HIS:O	1:A:39:CYS:HB2	1.88	0.73
1:C:242:LEU:HD22	1:D:80:LEU:HD22	1.70	0.73
1:A:220:THR:OG1	1:A:221:PRO:HD3	1.88	0.73
1:C:56:TYR:CD1	1:D:56:TYR:CD2	2.77	0.73
1:B:174:GLU:HA	1:B:191:LEU:HD22	1.71	0.73
1:B:306:ASN:ND2	1:B:306:ASN:H	1.87	0.73
1:A:259:ALA:HB1	1:B:265:ILE:HD13	1.70	0.72
1:A:90:GLU:OE2	1:B:49:ARG:NH2	2.23	0.72
1:B:146:TRP:CZ3	1:B:220:THR:HG22	2.23	0.72
1:C:104:ASN:HB3	1:C:255:HIS:CD2	2.24	0.72
1:B:50:ALA:HB1	1:B:102:LYS:HG3	1.71	0.72
1:B:57:GLY:HA2	1:B:60:LEU:HD12	1.70	0.72
1:D:251:ASP:O	1:D:255:HIS:CD2	2.43	0.72
1:A:21:GLU:HG3	1:A:22:VAL:HG22	1.70	0.71
1:C:284:LEU:CD1	1:D:239:GLU:HG3	2.20	0.71
1:C:284:LEU:HD11	1:D:239:GLU:HG3	1.72	0.71
1:B:143:GLN:HB2	1:B:227:MET:HE1	1.70	0.71
1:A:18:SER:O	1:A:24:ASN:ND2	2.22	0.71
1:A:300:PRO:HG3	1:B:150:MET:CE	2.19	0.71
1:B:31:ARG:NH2	1:B:235:GLN:HE21	1.89	0.70
1:B:49:ARG:NH1	1:B:53:GLU:OE2	2.23	0.70
1:A:68:ARG:HH21	1:A:89:THR:HG22	1.55	0.70
1:B:306:ASN:HB2	1:B:307:PRO:C	2.11	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:MET:CG	1:D:20:TRP:HB2	2.20	0.70
1:A:257:ASN:HD22	1:A:260:GLU:HB2	1.55	0.70
1:A:43:MET:HG2	1:A:113:VAL:HG21	1.73	0.70
1:D:31:ARG:HH22	1:D:235:GLN:HE21	1.38	0.70
1:C:239:GLU:HB2	1:D:284:LEU:HD11	1.74	0.70
1:D:33:ASP:OD2	1:D:132:THR:HG21	1.92	0.69
1:A:121:TYR:HB3	1:A:129:PHE:HE1	1.57	0.69
1:A:36:HIS:CE1	1:A:117:GLN:NE2	2.60	0.69
1:C:49:ARG:HG3	1:C:49:ARG:O	1.91	0.69
1:C:291:SER:HA	1:C:295:MET:HE1	1.74	0.69
1:A:183:VAL:HG13	1:A:184:THR:CG2	2.22	0.69
1:C:44:ASN:O	1:C:48:GLU:HG3	1.93	0.69
1:B:160:TYR:CE2	1:B:206:GLN:HB2	2.27	0.69
1:A:31:ARG:HH11	1:A:31:ARG:CG	2.05	0.69
1:D:22:VAL:HA	1:D:143:GLN:NE2	2.08	0.69
1:D:280:ALA:O	1:D:283:ASP:HB2	1.91	0.69
1:A:163:ALA:O	1:A:167:GLU:HB2	1.93	0.69
1:D:82:ARG:NH1	1:D:82:ARG:HG2	2.08	0.68
1:A:31:ARG:NH2	1:A:235:GLN:HG2	2.08	0.68
1:D:79:SER:HB3	1:D:283:ASP:OD1	1.94	0.68
1:A:75:PRO:HG2	1:B:38:LEU:HD21	1.74	0.68
1:B:60:LEU:HB2	1:B:95:SER:HB2	1.74	0.68
1:C:49:ARG:HB2	1:D:63:TRP:CZ2	2.28	0.68
1:C:184:THR:OG1	1:C:187:GLN:HB2	1.94	0.67
1:A:284:LEU:HD11	1:B:239:GLU:HB2	1.77	0.67
1:A:36:HIS:HB2	1:A:121:TYR:HE1	1.60	0.67
1:B:58:GLN:HA	1:B:58:GLN:HE21	1.60	0.67
1:C:87:ILE:HD12	1:C:87:ILE:N	2.08	0.67
1:A:126:MET:HA	1:A:127:GLY:O	1.94	0.67
1:C:293:PRO:HG3	1:D:19:PHE:CE1	2.30	0.67
1:C:293:PRO:HG3	1:D:19:PHE:HE1	1.61	0.66
1:A:144:LYS:HB3	1:A:145:PRO:HD3	1.76	0.66
1:A:31:ARG:HH11	1:A:31:ARG:HG2	1.60	0.66
1:A:44:ASN:H	1:A:44:ASN:HD22	1.43	0.66
1:C:54:LYS:HA	1:C:99:GLN:HE22	1.60	0.66
1:B:95:SER:O	1:B:99:GLN:HG2	1.96	0.66
1:C:144:LYS:HB3	1:C:145:PRO:HD3	1.76	0.66
1:C:98:HIS:CD2	1:C:258:LEU:HD11	2.31	0.66
1:A:43:MET:HE2	1:A:113:VAL:HG23	1.77	0.66
1:A:21:GLU:HG3	1:A:22:VAL:CG2	2.25	0.66
1:B:175:MET:SD	1:B:178:LYS:HD3	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TRP:CE3	1:A:117:GLN:HA	2.31	0.66
1:B:106:LEU:HD13	1:C:178:LYS:HB3	1.78	0.66
1:B:116:TRP:CH2	1:B:241:ARG:CB	2.78	0.65
1:B:144:LYS:HB3	1:B:145:PRO:CD	2.23	0.65
1:A:37:ARG:HH11	1:B:75:PRO:HD3	1.59	0.65
1:A:183:VAL:HG22	1:A:184:THR:HB	1.79	0.65
1:A:104:ASN:HB3	1:A:255:HIS:CD2	2.32	0.65
1:C:56:TYR:HD1	1:D:56:TYR:CB	2.09	0.65
1:A:253:LYS:HE3	1:B:272:GLU:HB2	1.79	0.65
1:B:273:GLN:HA	1:B:273:GLN:OE1	1.97	0.65
1:A:15:THR:HG22	1:A:16:THR:H	1.62	0.65
1:C:56:TYR:CD1	1:D:56:TYR:HB2	2.29	0.65
1:B:79:SER:HB2	1:B:278:ALA:HA	1.79	0.65
1:C:297:MET:HE2	1:D:21:GLU:N	2.12	0.65
1:A:76:GLN:HG3	1:A:81:GLU:HB3	1.78	0.65
1:B:22:VAL:HA	1:B:143:GLN:NE2	2.12	0.65
1:C:254:ARG:HB2	1:C:254:ARG:NH2	2.13	0.64
1:D:282:GLU:HA	1:D:285:ARG:HD2	1.78	0.64
1:C:220:THR:HB	1:C:221:PRO:HD3	1.79	0.64
1:A:66:ARG:NH1	1:B:48:GLU:OE1	2.31	0.64
1:C:259:ALA:HB2	1:D:264:TYR:CE2	2.32	0.64
1:C:261:ASN:HD22	1:C:261:ASN:C	2.00	0.64
1:C:19:PHE:H	1:D:295:MET:CE	2.08	0.64
1:A:183:VAL:HG22	1:A:184:THR:CA	2.28	0.64
1:A:179:THR:HG23	1:D:106:LEU:HD11	1.80	0.63
1:C:23:GLY:H	1:C:143:GLN:HE22	1.46	0.63
1:B:200:GLN:HB3	1:B:204:LYS:HE3	1.80	0.63
1:B:146:TRP:HZ3	1:B:220:THR:HG22	1.60	0.63
1:B:143:GLN:HB2	1:B:227:MET:HE2	1.79	0.63
1:A:303:GLU:HG3	1:B:157:LYS:NZ	2.14	0.63
1:A:264:TYR:HE2	1:B:259:ALA:H	1.47	0.62
1:D:36:HIS:O	1:D:39:CYS:HB2	1.99	0.62
1:B:31:ARG:NH2	1:B:235:GLN:NE2	2.48	0.62
1:B:110:LEU:C	1:B:110:LEU:HD13	2.19	0.62
1:A:209:TYR:HE1	1:B:302:PHE:HD2	1.45	0.62
1:D:122:HIS:H	1:D:130:LYS:HG3	1.64	0.62
1:C:136:GLU:HG2	1:C:140:ARG:HD2	1.81	0.62
1:D:88:MET:HE3	1:D:88:MET:N	2.15	0.61
1:A:43:MET:HG2	1:A:113:VAL:CG2	2.31	0.61
1:C:49:ARG:HB2	1:D:63:TRP:CE2	2.36	0.61
1:D:142:ALA:HB1	1:D:226:ASN:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:THR:O	1:A:32:ILE:HD13	2.01	0.61
1:A:31:ARG:HG2	1:A:31:ARG:NH1	2.15	0.61
1:A:85:GLY:HA2	1:A:88:MET:HE2	1.81	0.61
1:A:104:ASN:HB3	1:A:255:HIS:CG	2.36	0.61
1:D:236:GLN:HA	1:D:236:GLN:HE21	1.66	0.61
1:C:254:ARG:HH21	1:C:254:ARG:HG3	1.65	0.61
1:D:26:LYS:O	1:D:29:VAL:HG12	2.00	0.61
1:D:90:GLU:O	1:D:94:VAL:HG23	2.01	0.60
1:C:31:ARG:HE	1:C:238:GLU:HG2	1.66	0.60
1:B:245:LEU:O	1:B:245:LEU:HD22	2.01	0.60
1:D:76:GLN:HE21	1:D:76:GLN:CA	2.14	0.60
1:D:297:MET:HE3	1:D:297:MET:CA	2.30	0.60
1:C:264:TYR:OH	1:D:258:LEU:HB2	2.01	0.60
1:A:106:LEU:HD13	1:A:110:LEU:HD22	1.82	0.60
1:B:90:GLU:HG3	1:B:91:ALA:H	1.64	0.60
1:A:28:THR:HG22	1:B:287:PHE:CE1	2.35	0.60
1:A:36:HIS:HB2	1:A:121:TYR:CE1	2.36	0.60
1:D:141:LYS:HD2	1:D:141:LYS:N	2.17	0.60
1:C:57:GLY:O	1:C:61:THR:OG1	2.19	0.60
1:C:90:GLU:OE2	1:D:49:ARG:NH2	2.35	0.59
1:A:34:ASP:O	1:A:38:LEU:HD23	2.02	0.59
1:C:297:MET:HG3	1:D:20:TRP:CB	2.27	0.59
1:A:40:ASN:O	1:A:43:MET:HB2	2.03	0.59
1:D:26:LYS:NZ	1:D:30:LYS:HE3	2.17	0.59
1:A:110:LEU:O	1:A:110:LEU:HG	2.02	0.59
1:D:57:GLY:O	1:D:61:THR:HG23	2.02	0.59
1:B:251:ASP:HA	1:B:254:ARG:NH1	2.17	0.59
1:C:293:PRO:HB3	1:D:20:TRP:CZ2	2.37	0.59
1:A:253:LYS:HG3	1:A:254:ARG:N	2.17	0.59
1:C:165:LYS:HG3	1:D:305:TRP:CZ3	2.37	0.58
1:B:169:LEU:O	1:B:173:ARG:HB2	2.03	0.58
1:B:206:GLN:O	1:B:210:GLU:HB2	2.03	0.58
1:B:306:ASN:HD22	1:B:306:ASN:H	1.50	0.58
1:A:43:MET:HE2	1:A:114:LYS:CA	2.33	0.58
1:B:71:ILE:HD11	1:B:84:TRP:CH2	2.38	0.58
1:C:165:LYS:HG3	1:D:305:TRP:CH2	2.38	0.58
1:B:131:GLU:H	1:B:131:GLU:CD	2.07	0.58
1:A:31:ARG:HB3	1:A:31:ARG:HH11	1.68	0.58
1:A:101:VAL:O	1:A:105:LEU:HG	2.04	0.58
1:A:146:TRP:C	1:A:146:TRP:CD1	2.77	0.58
1:C:254:ARG:HH21	1:C:254:ARG:CG	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:THR:N	1:B:185:PRO:HD3	2.19	0.58
1:A:75:PRO:HG2	1:B:38:LEU:CD2	2.33	0.57
1:C:18:SER:HA	1:D:295:MET:CE	2.35	0.57
1:A:21:GLU:CG	1:A:22:VAL:HG22	2.34	0.57
1:C:216:VAL:HG11	1:D:300:PRO:HG2	1.86	0.57
1:D:56:TYR:HE1	1:D:60:LEU:HD21	1.69	0.57
1:A:19:PHE:CE1	1:B:293:PRO:HG3	2.33	0.57
1:A:243:VAL:CG1	1:A:244:PHE:N	2.66	0.57
1:D:297:MET:HE2	1:D:298:ASN:H	1.69	0.57
1:A:259:ALA:HB2	1:B:264:TYR:CD2	2.39	0.57
1:D:76:GLN:HE21	1:D:76:GLN:HA	1.69	0.57
1:A:295:MET:HE2	1:B:19:PHE:HB2	1.87	0.57
1:D:171:MET:O	1:D:175:MET:HB3	2.04	0.57
1:D:66:ARG:HH11	1:D:70:LEU:HD11	1.69	0.57
1:A:43:MET:CE	1:A:114:LYS:HA	2.35	0.57
1:C:267:VAL:HG13	1:C:268:TYR:CD2	2.40	0.57
1:A:69:GLN:O	1:A:72:GLU:HB3	2.04	0.56
1:A:45:CYS:HA	1:B:67:TRP:CE2	2.40	0.56
1:A:138:GLY:O	1:A:230:VAL:HG21	2.05	0.56
1:C:168:LYS:O	1:C:172:THR:HG23	2.05	0.56
1:C:75:PRO:HD2	1:D:38:LEU:HD21	1.86	0.56
1:A:35:GLY:HA3	1:A:241:ARG:HE	1.69	0.56
1:D:76:GLN:HG3	1:D:76:GLN:O	2.05	0.56
1:A:53:GLU:OE2	1:A:53:GLU:HA	2.04	0.56
1:A:81:GLU:HG3	1:A:82:ARG:H	1.71	0.56
1:D:281:GLN:O	1:D:284:LEU:HB2	2.05	0.56
1:B:177:SER:OG	1:B:191:LEU:HD11	2.05	0.56
1:B:184:THR:HB	1:B:187:GLN:HB3	1.88	0.56
1:B:44:ASN:O	1:B:48:GLU:HG3	2.05	0.56
1:C:197:LYS:O	1:C:200:GLN:HB3	2.06	0.56
1:A:168:LYS:HE2	1:A:172:THR:HG21	1.88	0.56
1:D:113:VAL:HG23	1:D:244:PHE:HE1	1.70	0.56
1:C:254:ARG:CZ	1:C:254:ARG:HB2	2.36	0.56
1:D:286:TRP:CH2	1:D:290:THR:HG21	2.41	0.56
1:A:81:GLU:CG	1:A:82:ARG:N	2.69	0.55
1:C:54:LYS:HA	1:C:99:GLN:NE2	2.20	0.55
1:B:176:ASN:O	1:B:179:THR:HG22	2.07	0.55
1:D:250:LEU:HD13	1:D:250:LEU:O	2.06	0.55
1:C:36:HIS:CE1	1:C:117:GLN:NE2	2.74	0.55
1:A:32:ILE:HG22	1:A:132:THR:HG23	1.89	0.55
1:A:124:GLN:C	1:A:125:ILE:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HD22	1:B:278:ALA:HB1	1.89	0.55
1:D:76:GLN:O	1:D:81:GLU:HB2	2.07	0.55
1:B:51:LYS:HG2	1:C:179:THR:OG1	2.07	0.55
1:A:49:ARG:HB2	1:B:63:TRP:CE2	2.42	0.55
1:B:228:GLU:O	1:B:228:GLU:HG3	2.06	0.55
1:D:292:GLY:O	1:D:295:MET:HG3	2.07	0.55
1:A:44:ASN:N	1:A:44:ASN:ND2	2.55	0.55
1:A:36:HIS:CE1	1:A:117:GLN:HE21	2.24	0.55
1:D:43:MET:SD	1:D:113:VAL:CG1	2.95	0.55
1:C:33:ASP:OD1	1:C:132:THR:HG21	2.06	0.54
1:A:120:ALA:O	1:A:121:TYR:CD2	2.60	0.54
1:A:15:THR:HG22	1:A:16:THR:N	2.21	0.54
1:C:60:LEU:HD22	1:D:52:ILE:HG21	1.88	0.54
1:A:80:LEU:HD11	1:B:246:LYS:HB2	1.89	0.54
1:A:31:ARG:HH11	1:A:31:ARG:CB	2.19	0.54
1:B:83:ALA:C	1:B:85:GLY:N	2.61	0.54
1:D:43:MET:HG3	1:D:113:VAL:HG11	1.89	0.54
1:A:35:GLY:CA	1:A:241:ARG:HE	2.21	0.54
1:B:157:LYS:HB2	1:B:209:TYR:HE1	1.72	0.54
1:C:297:MET:CE	1:D:21:GLU:HG2	2.38	0.54
1:A:257:ASN:HD21	1:A:260:GLU:HB2	1.71	0.54
1:C:261:ASN:ND2	1:C:263:SER:H	2.06	0.54
1:A:286:TRP:CE2	1:A:290:THR:HG21	2.42	0.54
1:C:56:TYR:O	1:C:60:LEU:HD23	2.08	0.53
1:C:87:ILE:H	1:C:87:ILE:CD1	2.20	0.53
1:C:239:GLU:O	1:C:243:VAL:HG23	2.08	0.53
1:B:83:ALA:C	1:B:85:GLY:H	2.10	0.53
1:D:37:ARG:O	1:D:40:ASN:N	2.42	0.53
1:D:82:ARG:NH1	1:D:82:ARG:CG	2.65	0.53
1:C:268:TYR:CE1	1:D:257:ASN:HA	2.43	0.53
1:C:38:LEU:HD21	1:D:75:PRO:HD2	1.89	0.53
1:A:122:HIS:HD2	1:A:131:GLU:OE2	1.92	0.53
1:B:110:LEU:C	1:B:110:LEU:CD1	2.77	0.53
1:A:56:TYR:CD1	1:B:56:TYR:HB2	2.42	0.53
1:A:266:HIS:CE1	1:A:270:GLU:HG3	2.44	0.53
1:A:175:MET:HE3	1:D:107:ASN:OD1	2.09	0.53
1:C:288:ARG:HH11	1:C:288:ARG:HG2	1.72	0.53
1:B:125:ILE:HG13	1:B:126:MET:N	2.24	0.53
1:A:182:SER:HB3	1:A:183:VAL:CG2	2.38	0.53
1:C:19:PHE:CD1	1:D:293:PRO:HA	2.44	0.53
1:C:143:GLN:HG3	1:C:223:TYR:OH	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:MET:CE	1:B:300:PRO:HG2	2.39	0.53
1:C:55:ALA:O	1:C:56:TYR:C	2.46	0.53
1:C:56:TYR:CD1	1:D:56:TYR:CG	2.97	0.53
1:D:56:TYR:CE1	1:D:60:LEU:HD21	2.43	0.53
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.02	0.52
1:A:146:TRP:CD1	1:A:146:TRP:O	2.62	0.52
1:A:183:VAL:HG22	1:A:184:THR:CB	2.39	0.52
1:A:37:ARG:NH1	1:B:75:PRO:HD3	2.24	0.52
1:C:138:GLY:C	1:C:230:VAL:HG21	2.30	0.52
1:A:156:ALA:O	1:A:209:TYR:HB2	2.09	0.52
1:A:53:GLU:OE2	1:B:56:TYR:OH	2.27	0.52
1:C:236:GLN:HA	1:C:236:GLN:HE21	1.74	0.52
1:C:284:LEU:HD12	1:D:239:GLU:HG3	1.92	0.52
1:C:288:ARG:NH1	1:C:288:ARG:HG2	2.23	0.52
1:A:79:SER:H	1:A:283:ASP:CG	2.12	0.52
1:A:216:VAL:O	1:A:220:THR:HG23	2.09	0.52
1:A:236:GLN:HE21	1:A:236:GLN:HA	1.74	0.52
1:D:245:LEU:HD22	1:D:249:LEU:HD12	1.92	0.52
1:C:183:VAL:HG13	1:C:187:GLN:HB3	1.91	0.52
1:B:31:ARG:HH22	1:B:235:GLN:NE2	1.97	0.52
1:D:43:MET:HG3	1:D:113:VAL:CG1	2.40	0.52
1:A:59:GLN:OE1	1:B:52:ILE:HG13	2.10	0.52
1:D:157:LYS:HB2	1:D:209:TYR:CE2	2.45	0.52
1:A:39:CYS:SG	1:A:116:TRP:CZ3	3.03	0.52
1:B:281:GLN:O	1:B:284:LEU:N	2.42	0.51
1:C:238:GLU:OE1	1:C:241:ARG:NH2	2.43	0.51
1:D:109:ASP:OD1	1:D:255:HIS:CD2	2.63	0.51
1:C:93:LYS:HD2	1:C:267:VAL:HG23	1.92	0.51
1:D:158:LYS:HB3	1:D:158:LYS:NZ	2.25	0.51
1:A:79:SER:N	1:A:283:ASP:OD2	2.43	0.51
1:B:133:LYS:HG3	1:B:137:ASP:OD2	2.10	0.51
1:B:38:LEU:HD12	1:B:241:ARG:NH1	2.25	0.51
1:A:271:LEU:HD22	1:A:275:ILE:CD1	2.41	0.51
1:D:104:ASN:OD1	1:D:255:HIS:ND1	2.43	0.51
1:C:261:ASN:HD22	1:C:263:SER:N	2.08	0.51
1:C:136:GLU:O	1:C:140:ARG:HG3	2.10	0.51
1:C:42:LEU:HD12	1:C:113:VAL:HG21	1.91	0.51
1:A:43:MET:HE2	1:A:114:LYS:N	2.24	0.51
1:C:78:GLY:O	1:C:81:GLU:HG2	2.11	0.51
1:B:157:LYS:HB2	1:B:209:TYR:CE1	2.45	0.51
1:B:71:ILE:HD11	1:B:84:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:TYR:HD2	1:B:98:HIS:CE1	2.28	0.51
1:D:151:LYS:HG3	1:D:152:GLU:N	2.25	0.51
1:A:184:THR:HG23	1:A:187:GLN:HB2	1.93	0.51
1:C:63:TRP:CZ2	1:D:49:ARG:HB2	2.45	0.51
1:C:66:ARG:O	1:C:70:LEU:HG	2.11	0.51
1:C:21:GLU:HB2	1:C:24:ASN:ND2	2.25	0.51
1:C:58:GLN:NE2	1:C:58:GLN:HA	2.21	0.51
1:A:36:HIS:CE1	1:A:129:PHE:CZ	2.99	0.51
1:B:177:SER:CB	1:B:191:LEU:HD11	2.41	0.51
1:A:253:LYS:HB2	1:B:271:LEU:HD13	1.92	0.51
1:D:76:GLN:C	1:D:76:GLN:HE21	2.14	0.51
1:A:182:SER:HB3	1:A:183:VAL:HG23	1.92	0.51
1:A:69:GLN:HE21	1:A:69:GLN:CA	2.23	0.50
1:D:29:VAL:CG1	1:D:30:LYS:N	2.75	0.50
1:C:267:VAL:HG13	1:C:268:TYR:N	2.26	0.50
1:A:67:TRP:O	1:A:68:ARG:C	2.49	0.50
1:C:25:TYR:O	1:C:28:THR:CG2	2.60	0.50
1:C:215:ASP:O	1:C:219:THR:HG23	2.12	0.50
1:A:160:TYR:CE1	1:A:206:GLN:HB2	2.47	0.50
1:A:221:PRO:HA	1:A:224:MET:HB2	1.93	0.50
1:A:45:CYS:HB2	1:B:67:TRP:CD2	2.45	0.50
1:B:76:GLN:HB3	1:B:81:GLU:HG3	1.93	0.50
1:B:291:SER:O	1:B:295:MET:CE	2.60	0.50
1:A:21:GLU:CD	1:A:22:VAL:HG22	2.32	0.50
1:A:105:LEU:HD11	1:A:256:LEU:HD11	1.92	0.50
1:C:113:VAL:HG12	1:C:113:VAL:O	2.11	0.50
1:D:110:LEU:C	1:D:110:LEU:HD23	2.32	0.50
1:B:238:GLU:OE2	1:B:238:GLU:HA	2.11	0.50
1:C:287:PHE:CE2	1:D:28:THR:HG22	2.46	0.50
1:A:76:GLN:HG3	1:A:77:TYR:N	2.27	0.50
1:A:33:ASP:CG	1:A:132:THR:HG21	2.32	0.50
1:A:43:MET:HE2	1:A:114:LYS:HA	1.93	0.50
1:B:306:ASN:HB2	1:B:308:ASP:N	2.27	0.50
1:C:131:GLU:H	1:C:131:GLU:CD	2.15	0.50
1:C:160:TYR:CE1	1:C:206:GLN:HB2	2.47	0.49
1:C:63:TRP:CE2	1:D:49:ARG:HB2	2.47	0.49
1:D:90:GLU:HG3	1:D:91:ALA:N	2.25	0.49
1:A:247:GLU:HG3	3:A:313:HOH:O	2.12	0.49
1:C:253:LYS:HB2	1:D:271:LEU:HD13	1.94	0.49
1:A:64:ALA:HA	1:A:88:MET:HG3	1.93	0.49
1:B:110:LEU:O	1:B:110:LEU:HD13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:SER:HA	1:D:295:MET:SD	2.51	0.49
1:D:63:TRP:CH2	1:D:88:MET:HE1	2.47	0.49
1:D:113:VAL:CG1	1:D:114:LYS:N	2.74	0.49
1:C:253:LYS:HD3	1:C:254:ARG:N	2.28	0.49
1:A:138:GLY:C	1:A:230:VAL:HG21	2.32	0.49
1:A:126:MET:N	1:A:127:GLY:HA3	2.27	0.49
1:D:214:GLU:O	1:D:218:LYS:HG3	2.13	0.49
1:A:121:TYR:HD1	1:A:129:PHE:CE1	2.31	0.49
1:A:76:GLN:HE21	1:A:77:TYR:H	1.59	0.49
1:A:47:GLN:O	1:A:51:LYS:HB2	2.13	0.49
1:B:146:TRP:CH2	1:B:220:THR:HG22	2.47	0.49
1:D:62:ASP:O	1:D:66:ARG:HB2	2.12	0.49
1:B:152:GLU:O	1:B:155:ALA:HB3	2.13	0.49
1:C:47:GLN:O	1:C:50:ALA:HB3	2.12	0.49
1:A:271:LEU:HD13	1:B:253:LYS:HB2	1.95	0.49
1:B:215:ASP:O	1:B:219:THR:HG22	2.13	0.49
1:B:50:ALA:O	1:B:51:LYS:C	2.50	0.49
1:D:64:ALA:HB2	1:D:91:ALA:HB3	1.95	0.49
1:D:110:LEU:HD23	1:D:111:GLU:N	2.28	0.49
1:A:36:HIS:CE1	1:A:129:PHE:HZ	2.31	0.48
1:C:257:ASN:OD1	1:D:268:TYR:CD2	2.66	0.48
1:D:76:GLN:NE2	1:D:76:GLN:HA	2.28	0.48
1:D:126:MET:HB2	1:D:127:GLY:HA2	1.96	0.48
1:A:31:ARG:HD3	1:B:287:PHE:CE2	2.48	0.48
1:B:279:ASP:OD2	1:B:281:GLN:HB2	2.14	0.48
1:D:76:GLN:NE2	1:D:76:GLN:CA	2.77	0.48
1:D:146:TRP:HZ3	1:D:220:THR:HA	1.78	0.48
1:C:245:LEU:HD22	1:C:249:LEU:HG	1.96	0.48
1:D:245:LEU:O	1:D:249:LEU:HB2	2.13	0.48
1:D:88:MET:HA	1:D:88:MET:CE	2.43	0.48
1:A:81:GLU:CG	1:A:82:ARG:H	2.25	0.48
1:B:154:GLU:O	1:B:158:LYS:HB2	2.13	0.48
1:D:128:GLY:HA3	1:D:133:LYS:HE2	1.95	0.48
1:B:258:LEU:O	1:B:261:ASN:CB	2.58	0.48
1:D:113:VAL:HG12	1:D:114:LYS:N	2.29	0.48
1:D:121:TYR:HA	1:D:130:LYS:CG	2.44	0.47
1:A:43:MET:HE3	1:A:113:VAL:HG23	1.94	0.47
1:C:245:LEU:HD12	1:D:80:LEU:HD23	1.95	0.47
1:C:261:ASN:O	1:C:262:SER:C	2.53	0.47
1:B:112:LYS:NZ	1:B:251:ASP:OD2	2.35	0.47
1:B:20:TRP:CZ3	1:B:224:MET:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:TRP:C	1:C:69:GLN:N	2.67	0.47
1:B:261:ASN:O	1:B:262:SER:C	2.53	0.47
1:A:42:LEU:O	1:A:43:MET:C	2.52	0.47
1:C:36:HIS:HB2	1:C:121:TYR:CE1	2.50	0.47
1:C:291:SER:HA	1:C:295:MET:CE	2.44	0.47
1:A:209:TYR:CE1	1:B:302:PHE:HD2	2.28	0.47
1:B:20:TRP:CZ3	1:B:224:MET:HG2	2.49	0.47
1:D:20:TRP:CZ3	1:D:224:MET:HA	2.49	0.47
1:A:39:CYS:O	1:A:43:MET:HG3	2.14	0.47
1:B:177:SER:HB3	1:B:191:LEU:HD11	1.96	0.47
1:B:259:ALA:C	1:B:261:ASN:H	2.17	0.47
1:B:306:ASN:ND2	1:B:306:ASN:N	2.61	0.47
1:A:45:CYS:HA	1:B:67:TRP:CZ2	2.49	0.47
1:A:150:MET:HE3	1:B:300:PRO:HG2	1.95	0.47
1:C:148:LYS:HE3	1:C:152:GLU:OE2	2.15	0.47
1:C:43:MET:HG2	1:C:110:LEU:HD12	1.97	0.47
1:D:54:LYS:O	1:D:58:GLN:HB2	2.15	0.47
1:C:56:TYR:CD1	1:D:56:TYR:CB	2.94	0.47
1:C:31:ARG:NE	1:C:238:GLU:HG2	2.29	0.47
1:C:78:GLY:C	1:C:80:LEU:H	2.19	0.47
1:D:238:GLU:OE1	1:D:241:ARG:NH1	2.48	0.47
1:A:241:ARG:CG	1:A:241:ARG:NH2	2.61	0.47
1:A:31:ARG:HH21	1:A:235:GLN:HG2	1.78	0.47
1:D:88:MET:HE3	1:D:88:MET:CA	2.45	0.47
1:C:257:ASN:HA	1:D:268:TYR:CZ	2.48	0.47
1:D:208:LYS:O	1:D:212:VAL:HG23	2.15	0.47
1:A:286:TRP:NE1	1:A:290:THR:HG21	2.30	0.47
1:D:200:GLN:HG2	1:D:204:LYS:HE3	1.97	0.47
1:B:259:ALA:C	1:B:261:ASN:N	2.68	0.46
1:B:265:ILE:H	1:B:265:ILE:HG12	1.58	0.46
1:C:104:ASN:CB	1:C:255:HIS:CD2	2.98	0.46
1:A:295:MET:CE	1:B:27:ARG:HH11	2.28	0.46
1:A:45:CYS:O	1:B:63:TRP:HZ2	1.98	0.46
1:C:272:GLU:HG3	1:D:250:LEU:HD21	1.97	0.46
1:A:102:LYS:HG2	1:A:103:ASN:N	2.27	0.46
1:B:107:ASN:ND2	1:C:175:MET:HE1	2.29	0.46
1:C:49:ARG:HD3	1:D:63:TRP:CZ3	2.51	0.46
1:A:52:ILE:HG12	1:B:59:GLN:NE2	2.31	0.46
1:A:143:GLN:O	1:A:147:ALA:N	2.49	0.46
1:C:56:TYR:HD1	1:D:56:TYR:CG	2.33	0.46
1:A:69:GLN:NE2	1:A:69:GLN:HA	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:HG3	1:B:305:TRP:HZ2	1.80	0.46
1:B:281:GLN:O	1:B:282:GLU:C	2.53	0.46
1:C:184:THR:OG1	1:C:187:GLN:CB	2.63	0.46
1:C:261:ASN:ND2	1:C:261:ASN:C	2.64	0.46
1:D:167:GLU:HB2	1:D:202:VAL:HG21	1.96	0.46
1:C:25:TYR:OH	1:C:140:ARG:HG2	2.16	0.46
1:D:89:THR:O	1:D:90:GLU:C	2.54	0.46
1:A:143:GLN:HA	1:A:223:TYR:HE1	1.80	0.46
1:C:190:LYS:HE2	1:C:194:LYS:HE3	1.98	0.46
1:C:229:GLN:HB3	1:C:229:GLN:HE21	1.55	0.46
1:A:66:ARG:HH12	1:B:48:GLU:CD	2.19	0.45
1:D:236:GLN:HA	1:D:236:GLN:NE2	2.30	0.45
1:C:265:ILE:HD13	1:D:259:ALA:HB2	1.98	0.45
1:C:174:GLU:HA	1:C:191:LEU:HD23	1.98	0.45
1:B:252:ILE:O	1:B:253:LYS:C	2.52	0.45
1:B:51:LYS:HE2	1:B:51:LYS:HB3	1.72	0.45
1:C:31:ARG:NH2	1:C:235:GLN:NE2	2.64	0.45
1:C:80:LEU:HD13	1:D:245:LEU:CD1	2.46	0.45
1:D:113:VAL:HG23	1:D:244:PHE:CE1	2.51	0.45
1:B:104:ASN:O	1:B:105:LEU:C	2.51	0.45
1:D:88:MET:CA	1:D:88:MET:CE	2.94	0.45
1:A:116:TRP:CE3	1:A:117:GLN:CA	2.99	0.45
1:A:22:VAL:HB	1:A:23:GLY:H	1.20	0.45
1:A:253:LYS:HB2	1:B:271:LEU:CD1	2.46	0.45
1:A:232:GLU:O	1:A:236:GLN:HB2	2.17	0.45
1:B:39:CYS:O	1:B:40:ASN:C	2.54	0.45
1:C:56:TYR:CE1	1:D:56:TYR:CD2	3.05	0.45
1:C:184:THR:HB	1:C:185:PRO:HD2	1.97	0.45
1:C:25:TYR:O	1:C:28:THR:HG23	2.17	0.45
1:C:66:ARG:O	1:C:69:GLN:HB3	2.16	0.45
1:A:264:TYR:OH	1:B:258:LEU:HB2	2.17	0.45
1:C:157:LYS:O	1:C:158:LYS:C	2.53	0.45
1:A:116:TRP:HE3	1:A:117:GLN:N	2.14	0.45
1:C:54:LYS:HB2	1:C:102:LYS:HD3	1.98	0.45
1:D:43:MET:SD	1:D:113:VAL:HG13	2.57	0.45
1:D:238:GLU:O	1:D:241:ARG:N	2.47	0.45
1:D:307:PRO:O	1:D:308:ASP:C	2.54	0.45
1:A:297:MET:SD	1:A:298:ASN:N	2.89	0.45
1:C:68:ARG:O	1:C:72:GLU:HB2	2.17	0.45
1:D:248:VAL:O	1:D:251:ASP:HB2	2.17	0.45
1:A:303:GLU:HG3	1:B:157:LYS:HZ2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:HB2	1:A:278:ALA:HA	1.99	0.45
1:C:287:PHE:HE2	1:D:28:THR:HG22	1.81	0.45
1:D:238:GLU:HA	1:D:238:GLU:OE2	2.17	0.45
1:C:276:ARG:HA	1:D:246:LYS:HE2	1.99	0.45
1:D:49:ARG:NH1	1:D:53:GLU:OE2	2.48	0.45
1:A:251:ASP:OD1	1:A:254:ARG:NH1	2.47	0.45
1:B:24:ASN:C	1:B:26:LYS:N	2.69	0.45
1:D:26:LYS:HZ1	1:D:30:LYS:HE3	1.80	0.45
1:A:83:ALA:O	1:A:86:ALA:HB3	2.17	0.45
1:D:297:MET:HE2	1:D:298:ASN:N	2.31	0.44
1:D:284:LEU:HA	1:D:284:LEU:HD23	1.70	0.44
1:C:80:LEU:HD12	1:D:242:LEU:HD22	1.98	0.44
1:B:139:PHE:HD1	1:B:227:MET:SD	2.40	0.44
1:B:101:VAL:O	1:B:102:LYS:C	2.53	0.44
1:A:300:PRO:HG3	1:B:150:MET:HE1	1.99	0.44
1:A:66:ARG:NH1	1:B:48:GLU:CD	2.71	0.44
1:B:37:ARG:O	1:B:40:ASN:HB2	2.17	0.44
1:B:90:GLU:CG	1:B:91:ALA:N	2.62	0.44
1:C:275:ILE:C	1:C:277:GLY:N	2.70	0.44
1:B:174:GLU:HG3	1:B:191:LEU:HB3	2.00	0.44
1:A:122:HIS:CD2	1:A:131:GLU:OE2	2.70	0.44
1:A:125:ILE:C	1:A:127:GLY:HA3	2.38	0.44
1:C:261:ASN:HD22	1:C:263:SER:H	1.65	0.44
1:A:102:LYS:O	1:A:103:ASN:C	2.56	0.44
1:A:241:ARG:C	1:A:243:VAL:N	2.68	0.44
1:B:153:LEU:HD11	1:B:213:LEU:HD23	1.99	0.44
1:C:242:LEU:O	1:C:243:VAL:C	2.55	0.44
1:B:83:ALA:O	1:B:85:GLY:N	2.51	0.44
1:C:275:ILE:C	1:C:277:GLY:H	2.21	0.44
1:C:181:GLN:HA	1:C:182:SER:HA	1.58	0.44
1:D:140:ARG:NH1	1:D:140:ARG:CG	2.63	0.44
1:C:56:TYR:CE1	1:D:56:TYR:HD2	2.35	0.44
1:A:36:HIS:ND1	1:A:121:TYR:CD1	2.85	0.44
1:C:235:GLN:HG3	1:D:288:ARG:NH2	2.33	0.44
1:B:107:ASN:O	1:B:111:GLU:HB2	2.17	0.44
1:A:189:LYS:HD2	1:A:189:LYS:HA	1.71	0.44
1:A:281:GLN:NE2	1:B:239:GLU:OE1	2.51	0.44
1:D:26:LYS:HZ3	1:D:30:LYS:HE3	1.82	0.44
1:A:25:TYR:CD1	1:A:139:PHE:HB3	2.53	0.44
1:B:109:ASP:O	1:B:110:LEU:C	2.55	0.43
1:A:19:PHE:HA	1:A:24:ASN:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:GLU:OE1	1:C:242:LEU:HD21	2.18	0.43
1:A:157:LYS:CB	1:A:209:TYR:CE2	3.01	0.43
1:C:231:PHE:O	1:C:234:CYS:HB2	2.18	0.43
1:D:297:MET:CE	1:D:298:ASN:H	2.31	0.43
1:A:165:LYS:HG3	1:B:305:TRP:CZ2	2.54	0.43
1:C:150:MET:CE	1:D:300:PRO:HG3	2.48	0.43
1:B:280:ALA:O	1:B:283:ASP:HB2	2.17	0.43
1:C:297:MET:HE2	1:D:21:GLU:HG2	2.01	0.43
1:C:18:SER:HA	1:D:295:MET:HE3	1.99	0.43
1:B:291:SER:O	1:B:295:MET:HE2	2.18	0.43
1:A:300:PRO:HB3	1:B:153:LEU:HD21	2.01	0.43
1:C:98:HIS:CD2	1:C:258:LEU:CD1	2.99	0.43
1:C:272:GLU:HB2	1:D:253:LYS:HE3	2.00	0.43
1:B:47:GLN:HA	1:B:106:LEU:HD21	2.00	0.43
1:B:97:LEU:O	1:B:100:GLU:N	2.50	0.43
1:B:31:ARG:O	1:B:34:ASP:HB2	2.18	0.43
1:D:67:TRP:HB3	1:D:88:MET:SD	2.59	0.43
1:A:291:SER:C	1:A:295:MET:HE2	2.39	0.43
1:B:207:GLU:O	1:B:211:LYS:HB2	2.19	0.43
1:D:252:ILE:O	1:D:253:LYS:C	2.56	0.43
1:C:131:GLU:CD	1:C:131:GLU:N	2.71	0.43
1:C:20:TRP:CZ3	1:C:224:MET:HA	2.54	0.43
1:B:160:TYR:CD1	1:B:160:TYR:C	2.92	0.43
1:A:71:ILE:HD13	1:A:71:ILE:C	2.39	0.43
1:C:266:HIS:C	1:C:266:HIS:CD2	2.92	0.43
1:A:258:LEU:O	1:A:261:ASN:N	2.47	0.43
1:C:157:LYS:O	1:C:160:TYR:N	2.52	0.43
1:B:49:ARG:O	1:B:50:ALA:C	2.57	0.43
1:A:116:TRP:CE3	1:A:117:GLN:N	2.87	0.43
1:C:272:GLU:HG2	1:C:272:GLU:O	2.19	0.43
1:C:232:GLU:O	1:C:236:GLN:HG2	2.19	0.43
1:A:183:VAL:CG2	1:A:184:THR:HB	2.48	0.42
1:C:98:HIS:NE2	1:C:258:LEU:CD1	2.82	0.42
1:C:270:GLU:HA	1:C:273:GLN:HB3	2.01	0.42
1:A:183:VAL:HG13	1:A:184:THR:CB	2.48	0.42
1:A:50:ALA:HB2	1:A:105:LEU:HB3	2.00	0.42
1:C:32:ILE:CG2	1:C:132:THR:HG22	2.49	0.42
1:B:213:LEU:O	1:B:216:VAL:HG12	2.20	0.42
1:B:187:GLN:O	1:B:191:LEU:HG	2.19	0.42
1:D:305:TRP:O	1:D:305:TRP:CD1	2.72	0.42
1:A:44:ASN:HA	1:A:47:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LYS:HZ3	1:D:30:LYS:HG3	1.85	0.42
1:A:297:MET:HB3	1:A:299:TRP:NE1	2.35	0.42
1:A:19:PHE:CE1	1:B:293:PRO:HD3	2.53	0.42
1:C:245:LEU:CD1	1:D:80:LEU:HD23	2.49	0.42
1:D:88:MET:H	1:D:88:MET:HG2	1.63	0.42
1:B:285:ARG:O	1:B:286:TRP:C	2.57	0.42
1:C:245:LEU:O	1:C:249:LEU:HG	2.19	0.42
1:A:76:GLN:HB2	1:B:38:LEU:HD13	2.02	0.42
1:A:264:TYR:CE2	1:B:259:ALA:HB2	2.54	0.42
1:B:291:SER:C	1:B:295:MET:CE	2.88	0.42
1:C:254:ARG:CB	1:C:254:ARG:NH2	2.83	0.42
1:C:102:LYS:HE2	1:C:102:LYS:HB3	1.71	0.42
1:A:209:TYR:HE1	1:B:302:PHE:CD2	2.33	0.42
1:A:306:ASN:HA	1:A:307:PRO:HD3	1.91	0.42
1:D:118:LYS:HD2	1:D:118:LYS:HA	1.83	0.42
1:C:52:ILE:HD13	1:D:59:GLN:HB3	2.02	0.42
1:A:271:LEU:HD22	1:A:275:ILE:HD11	2.02	0.42
1:C:254:ARG:CG	1:C:254:ARG:NH2	2.78	0.42
1:C:75:PRO:O	1:C:77:TYR:HD1	2.02	0.42
1:A:143:GLN:HA	1:A:223:TYR:CE1	2.54	0.42
1:B:46:VAL:HG13	1:B:105:LEU:HB3	2.02	0.42
1:D:44:ASN:O	1:D:45:CYS:C	2.58	0.42
1:A:116:TRP:HE3	1:A:117:GLN:CA	2.33	0.42
1:D:63:TRP:CZ3	1:D:88:MET:HE2	2.55	0.42
1:B:157:LYS:N	1:B:209:TYR:CD1	2.88	0.42
1:A:157:LYS:HA	1:A:209:TYR:CD2	2.55	0.42
1:B:245:LEU:C	1:B:245:LEU:HD22	2.40	0.42
1:B:280:ALA:HA	1:B:283:ASP:HB2	2.01	0.42
1:B:35:GLY:HA3	1:B:121:TYR:OH	2.20	0.42
1:C:281:GLN:HG2	1:C:281:GLN:H	1.62	0.42
1:C:157:LYS:HG2	1:C:209:TYR:CZ	2.55	0.41
1:A:31:ARG:HH22	1:A:235:GLN:HG2	1.84	0.41
1:A:43:MET:HE1	1:A:114:LYS:HA	2.02	0.41
1:A:157:LYS:HG3	1:A:158:LYS:N	2.35	0.41
1:A:80:LEU:HD12	1:B:245:LEU:CD1	2.50	0.41
1:D:151:LYS:HE2	1:D:151:LYS:HB2	1.94	0.41
1:A:307:PRO:O	1:A:308:ASP:C	2.58	0.41
1:A:295:MET:HE1	1:B:27:ARG:HH11	1.86	0.41
1:B:67:TRP:HB3	1:B:88:MET:HE1	2.01	0.41
1:B:167:GLU:O	1:B:171:MET:HB2	2.20	0.41
1:C:26:LYS:HA	1:C:29:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:CG2	1:A:184:THR:HA	2.44	0.41
1:C:81:GLU:HG3	1:C:82:ARG:N	2.35	0.41
1:D:37:ARG:HD3	1:D:41:ASP:OD2	2.21	0.41
1:A:174:GLU:O	1:A:178:LYS:HG3	2.21	0.41
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.76	0.41
1:C:101:VAL:O	1:C:105:LEU:HG	2.20	0.41
1:C:87:ILE:HG22	1:C:87:ILE:O	2.21	0.41
1:A:303:GLU:HG3	1:B:157:LYS:HZ3	1.85	0.41
1:A:295:MET:CE	1:B:19:PHE:HB2	2.50	0.41
1:A:122:HIS:H	1:A:122:HIS:CD2	2.37	0.41
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.82	0.41
1:D:18:SER:O	1:D:21:GLU:HB2	2.20	0.41
1:D:248:VAL:CG1	1:D:249:LEU:N	2.84	0.41
1:A:284:LEU:CD1	1:B:239:GLU:HB2	2.49	0.41
1:A:15:THR:CG2	1:A:16:THR:H	2.30	0.41
1:C:25:TYR:O	1:C:28:THR:HG22	2.21	0.41
1:C:64:ALA:HB2	1:C:91:ALA:HB3	2.03	0.41
1:A:20:TRP:HD1	1:B:297:MET:HB2	1.85	0.41
1:D:57:GLY:O	1:D:61:THR:CG2	2.69	0.41
1:C:150:MET:HE1	1:D:300:PRO:HG3	2.03	0.41
1:B:21:GLU:HB2	1:B:24:ASN:ND2	2.36	0.41
1:A:50:ALA:HB2	1:A:105:LEU:CD1	2.51	0.41
1:D:111:GLU:O	1:D:112:LYS:C	2.59	0.41
1:C:86:ALA:HB1	1:C:271:LEU:HD22	2.02	0.41
1:D:122:HIS:HD2	1:D:130:LYS:HG2	1.86	0.41
1:C:250:LEU:CD1	1:C:254:ARG:HH12	2.24	0.41
1:C:245:LEU:HD23	1:C:245:LEU:HA	1.73	0.41
1:C:284:LEU:HD23	1:C:284:LEU:HA	1.80	0.41
1:A:165:LYS:C	1:A:167:GLU:N	2.74	0.41
1:A:165:LYS:C	1:A:167:GLU:H	2.24	0.41
1:C:22:VAL:HA	1:C:143:GLN:NE2	2.36	0.41
1:B:67:TRP:CZ3	1:B:70:LEU:HD12	2.56	0.41
1:B:93:LYS:HD3	1:B:267:VAL:HG22	2.02	0.41
1:A:80:LEU:HD12	1:B:245:LEU:HD13	2.03	0.41
1:A:106:LEU:N	1:A:106:LEU:CD2	2.84	0.41
1:D:146:TRP:O	1:D:146:TRP:CD1	2.74	0.41
1:B:162:LEU:O	1:B:166:GLU:HG2	2.21	0.41
1:B:192:GLN:HG2	1:B:192:GLN:O	2.21	0.41
1:B:248:VAL:O	1:B:251:ASP:HB2	2.20	0.40
1:C:129:PHE:HB2	1:C:132:THR:HG23	2.03	0.40
1:D:51:LYS:O	1:D:52:ILE:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLU:CB	1:D:284:LEU:HD11	2.48	0.40
1:A:20:TRP:CZ3	1:A:224:MET:HA	2.56	0.40
1:C:45:CYS:HA	1:D:67:TRP:CZ2	2.56	0.40
1:D:253:LYS:HD3	1:D:254:ARG:N	2.36	0.40
1:A:149:LYS:HE3	1:A:219:THR:HG21	2.02	0.40
1:D:271:LEU:O	1:D:274:ALA:N	2.54	0.40
1:D:260:GLU:O	1:D:260:GLU:HG3	2.22	0.40
1:D:121:TYR:HA	1:D:130:LYS:HG2	2.03	0.40
1:D:55:ALA:O	1:D:56:TYR:C	2.59	0.40
1:B:291:SER:O	1:B:295:MET:HE1	2.21	0.40
1:A:148:LYS:HA	1:A:148:LYS:HD2	1.84	0.40
1:A:31:ARG:HD2	1:B:77:TYR:OH	2.22	0.40
1:A:21:GLU:O	1:A:22:VAL:C	2.59	0.40
1:C:93:LYS:O	1:C:97:LEU:HD23	2.21	0.40
1:A:168:LYS:HE2	1:A:172:THR:CG2	2.50	0.40
1:B:117:GLN:HG2	1:B:117:GLN:O	2.20	0.40
1:A:240:LYS:HE2	1:A:240:LYS:HA	2.02	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	292/308 (95%)	254 (87%)	31 (11%)	7 (2%)	7	27
1	B	292/308 (95%)	256 (88%)	32 (11%)	4 (1%)	14	42
1	C	283/308 (92%)	259 (92%)	23 (8%)	1 (0%)	39	73
1	D	272/308 (88%)	246 (90%)	25 (9%)	1 (0%)	39	73
All	All	1139/1232 (92%)	1015 (89%)	111 (10%)	13 (1%)	17	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	D	52	ILE
1	A	104	ASN
1	A	281	GLN
1	B	31	ARG
1	B	281	GLN
1	B	84	TRP
1	B	134	GLU
1	C	281	GLN
1	A	18	SER
1	A	48	GLU
1	A	254	ARG
1	A	127	GLY

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	261/274 (95%)	218 (84%)	43 (16%)	3	7
1	B	260/274 (95%)	234 (90%)	26 (10%)	9	26
1	C	252/274 (92%)	226 (90%)	26 (10%)	9	24
1	D	241/274 (88%)	209 (87%)	32 (13%)	5	13
All	All	1014/1096 (92%)	887 (88%)	127 (12%)	6	15

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

Mol	Chain	Res	Type
1	A	19	PHE
1	A	22	VAL
1	A	25	TYR
1	A	29	VAL
1	A	31	ARG
1	A	42	LEU
1	A	44	ASN
1	A	45	CYS
1	A	49	ARG

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Mol	Chain	Res	Type
1	A	51	LYS
1	A	52	ILE
1	A	61	THR
1	A	69	GLN
1	A	71	ILE
1	A	89	THR
1	A	90	GLU
1	A	106	LEU
1	A	126	MET
1	A	132	THR
1	A	134	GLU
1	A	146	TRP
1	A	148	LYS
1	A	151	LYS
1	A	161	HIS
1	A	162	LEU
1	A	166	GLU
1	A	167	GLU
1	A	180	GLU
1	A	184	THR
1	A	192	GLN
1	A	208	LYS
1	A	215	ASP
1	A	232	GLU
1	A	236	GLN
1	A	240	LYS
1	A	241	ARG
1	A	243	VAL
1	A	245	LEU
1	A	253	LYS
1	A	260	GLU
1	A	271	LEU
1	A	272	GLU
1	A	306	ASN
1	B	28	THR
1	B	31	ARG
1	B	42	LEU
1	B	49	ARG
1	B	70	LEU
1	B	88	MET
1	B	90	GLU
1	B	108	GLU

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Mol	Chain	Res	Type
1	B	125	ILE
1	B	131	GLU
1	B	134	GLU
1	B	140	ARG
1	B	141	LYS
1	B	158	LYS
1	B	161	HIS
1	B	175	MET
1	B	178	LYS
1	B	179	THR
1	B	213	LEU
1	B	216	VAL
1	B	219	THR
1	B	240	LYS
1	B	245	LEU
1	B	265	ILE
1	B	271	LEU
1	B	306	ASN
1	C	28	THR
1	C	31	ARG
1	C	37	ARG
1	C	58	GLN
1	C	61	THR
1	C	71	ILE
1	C	90	GLU
1	C	126	MET
1	C	141	LYS
1	C	150	MET
1	C	151	LYS
1	C	162	LEU
1	C	179	THR
1	C	181	GLN
1	C	225	GLU
1	C	226	ASN
1	C	229	GLN
1	C	236	GLN
1	C	245	LEU
1	C	250	LEU
1	C	251	ASP
1	C	254	ARG
1	C	261	ASN
1	C	271	LEU

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Mol	Chain	Res	Type
1	C	297	MET
1	C	299	TRP
1	D	29	VAL
1	D	31	ARG
1	D	37	ARG
1	D	43	MET
1	D	58	GLN
1	D	61	THR
1	D	66	ARG
1	D	76	GLN
1	D	79	SER
1	D	82	ARG
1	D	88	MET
1	D	90	GLU
1	D	97	LEU
1	D	98	HIS
1	D	99	GLN
1	D	113	VAL
1	D	125	ILE
1	D	130	LYS
1	D	140	ARG
1	D	151	LYS
1	D	161	HIS
1	D	167	GLU
1	D	225	GLU
1	D	226	ASN
1	D	229	GLN
1	D	236	GLN
1	D	245	LEU
1	D	248	VAL
1	D	251	ASP
1	D	271	LEU
1	D	297	MET
1	D	305	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	GLN
1	A	76	GLN
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	117	GLN
1	A	122	HIS
1	A	206	GLN
1	A	222	GLN
1	A	236	GLN
1	A	257	ASN
1	A	261	ASN
1	A	266	HIS
1	B	44	ASN
1	B	58	GLN
1	B	69	GLN
1	B	206	GLN
1	B	222	GLN
1	B	235	GLN
1	B	236	GLN
1	B	306	ASN
1	C	44	ASN
1	C	58	GLN
1	C	99	GLN
1	C	103	ASN
1	C	143	GLN
1	C	181	GLN
1	C	200	GLN
1	C	206	GLN
1	C	222	GLN
1	C	226	ASN
1	C	229	GLN
1	C	235	GLN
1	C	236	GLN
1	C	255	HIS
1	C	261	ASN
1	C	266	HIS
1	D	36	HIS
1	D	69	GLN
1	D	76	GLN
1	D	122	HIS
1	D	124	GLN
1	D	143	GLN
1	D	222	GLN
1	D	229	GLN
1	D	235	GLN
1	D	236	GLN

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Mol	Chain	Res	Type
1	D	281	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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	294/308 (95%)	0.50	12 (4%) 41 35	43, 74, 116, 166	0
1	B	294/308 (95%)	0.45	14 (4%) 34 29	35, 66, 137, 168	0
1	C	285/308 (92%)	0.39	12 (4%) 40 34	55, 80, 118, 153	0
1	D	276/308 (89%)	0.68	31 (11%) 7 4	60, 85, 202, 232	0
All	All	1149/1232 (93%)	0.50	69 (6%) 25 19	35, 78, 151, 232	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	209	TYR	7.5
1	D	213	LEU	6.6
1	D	198	CYS	5.0
1	D	260	GLU	4.9
1	D	202	VAL	4.9
1	D	172	THR	4.5
1	C	27	ARG	4.5
1	D	168	LYS	4.4
1	B	180	GLU	4.2
1	B	191	LEU	4.2
1	D	211	LYS	4.1
1	A	27	ARG	4.1
1	C	77	TYR	4.0
1	B	187	GLN	3.9
1	D	166	GLU	3.8
1	C	203	GLN	3.6
1	D	27	ARG	3.6
1	D	214	GLU	3.4
1	B	195	VAL	3.4
1	D	200	GLN	3.3
1	A	305	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	183	VAL	3.2
1	B	197	LYS	3.2
1	D	208	LYS	3.2
1	C	204	LYS	3.1
1	D	204	LYS	2.9
1	D	300	PRO	2.9
1	A	209	TYR	2.9
1	B	293	PRO	2.8
1	D	216	VAL	2.8
1	A	183	VAL	2.7
1	D	199	LYS	2.7
1	C	258	LEU	2.6
1	A	19	PHE	2.6
1	C	293	PRO	2.6
1	D	152	GLU	2.5
1	D	149	LYS	2.5
1	D	207	GLU	2.4
1	C	298	ASN	2.4
1	C	211	LYS	2.4
1	D	258	LEU	2.3
1	A	179	THR	2.3
1	D	231	PHE	2.3
1	A	22	VAL	2.3
1	D	154	GLU	2.3
1	D	77	TYR	2.3
1	A	154	GLU	2.3
1	C	300	PRO	2.2
1	A	260	GLU	2.2
1	A	125	ILE	2.2
1	B	299	TRP	2.2
1	C	292	GLY	2.2
1	D	203	GLN	2.2
1	B	200	GLN	2.2
1	B	213	LEU	2.2
1	B	27	ARG	2.2
1	D	197	LYS	2.1
1	D	220	THR	2.1
1	C	265	ILE	2.1
1	B	184	THR	2.1
1	D	169	LEU	2.1
1	D	163	ALA	2.1
1	D	298	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	124	GLN	2.1
1	A	304	GLU	2.0
1	B	204	LYS	2.0
1	D	161	HIS	2.0
1	B	301	GLN	2.0
1	C	192	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	310	1/1	0.71	0.28	2.10	102,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.