Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:15 AM GMT

PDB ID	:	3HNP
Title	:	Crystal Structure of an Oxidoreductase from Bacillus cereus. Northeast Structural Genomics Consortium target id BcR251
Authors	:	Seetharaman, J.; Su, M.; Sahdev, S.; Janjua, H.; Xiao, R.; Ciccosanti, C.; Foote, E.L.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-05-31
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

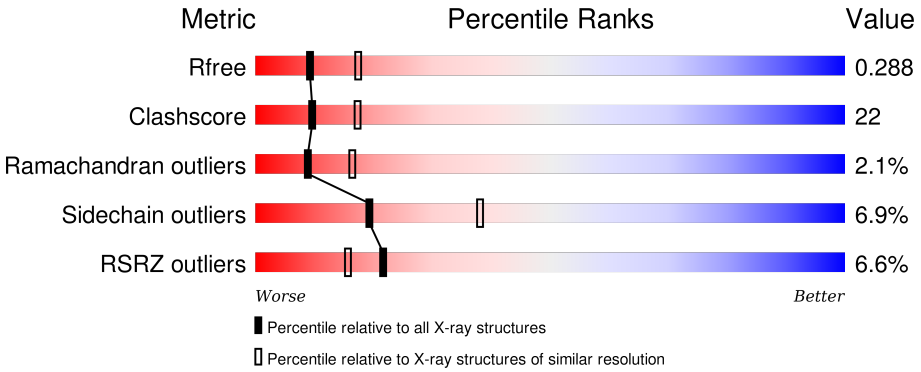
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	353	62% 35%
1	B	353	56% 40%
1	C	353	8% 56% 37%
1	D	353	6% 51% 44%
1	E	353	8% 48% 30% 6% 16%

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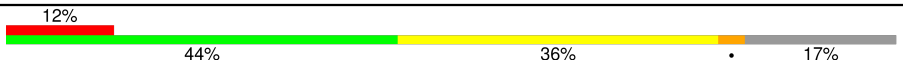
Mol	Chain	Length	Quality of chain
1	F	353	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15535 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 Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2767	1772	466	521	8			
1	B	350	Total	C	N	O	S	0	0	0
			2777	1778	468	523	8			
1	C	340	Total	C	N	O	S	0	0	0
			2667	1709	449	501	8			
1	D	344	Total	C	N	O	S	0	0	0
			2731	1749	458	516	8			
1	E	297	Total	C	N	O	S	0	0	0
			2299	1465	387	440	7			
1	F	294	Total	C	N	O	S	0	0	0
			2205	1401	376	422	6			

- Molecule 2 is water.

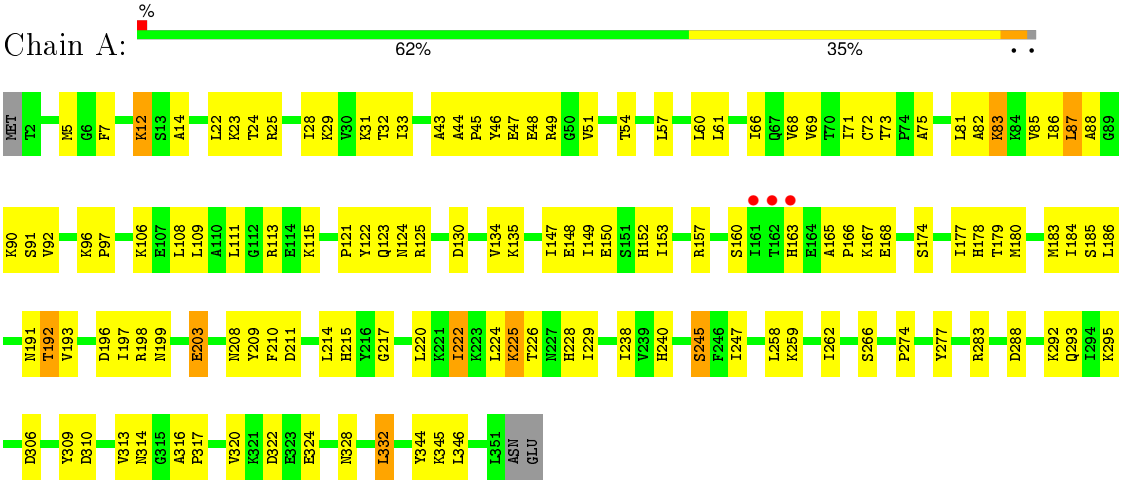
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		
2	B	12	Total	O	0	0
			12	12		
2	C	6	Total	O	0	0
			6	6		
2	D	10	Total	O	0	0
			10	10		
2	E	17	Total	O	0	0
			17	17		
2	F	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

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

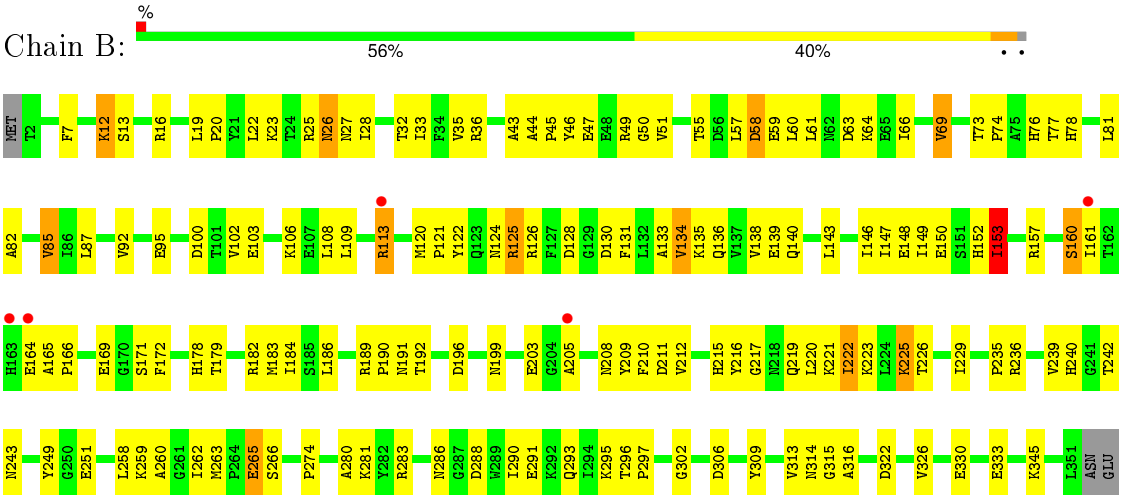
- Molecule 1: Oxidoreductase

Chain A:



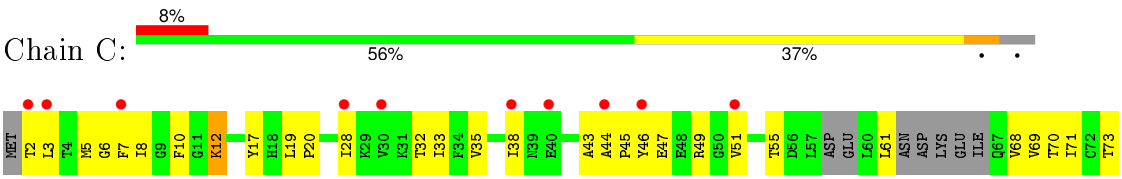
- Molecule 1: Oxidoreductase

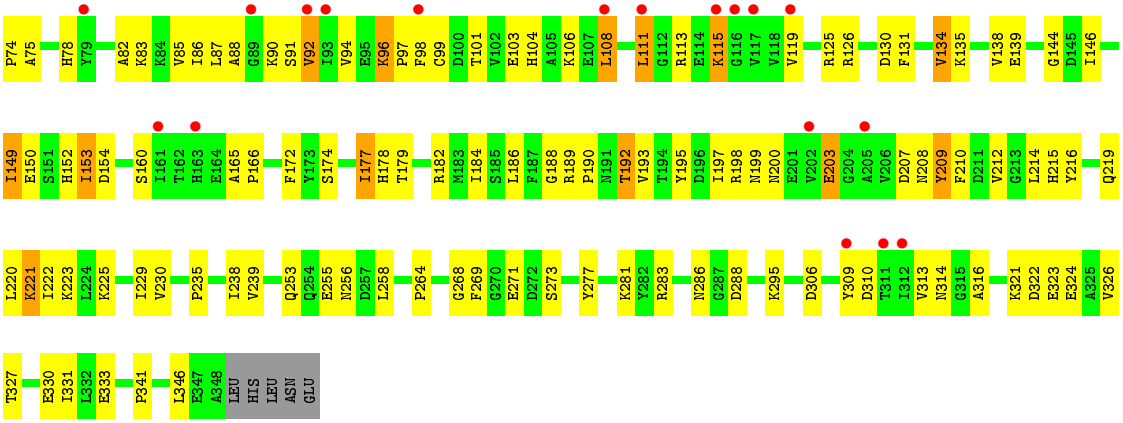
Chain B:



- Molecule 1: Oxidoreductase

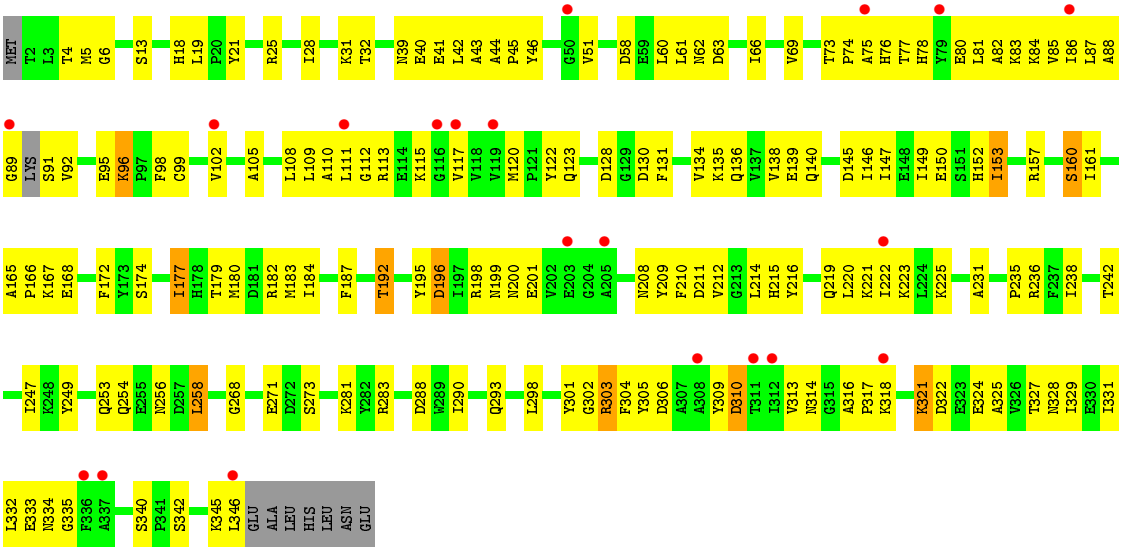
Chain C:





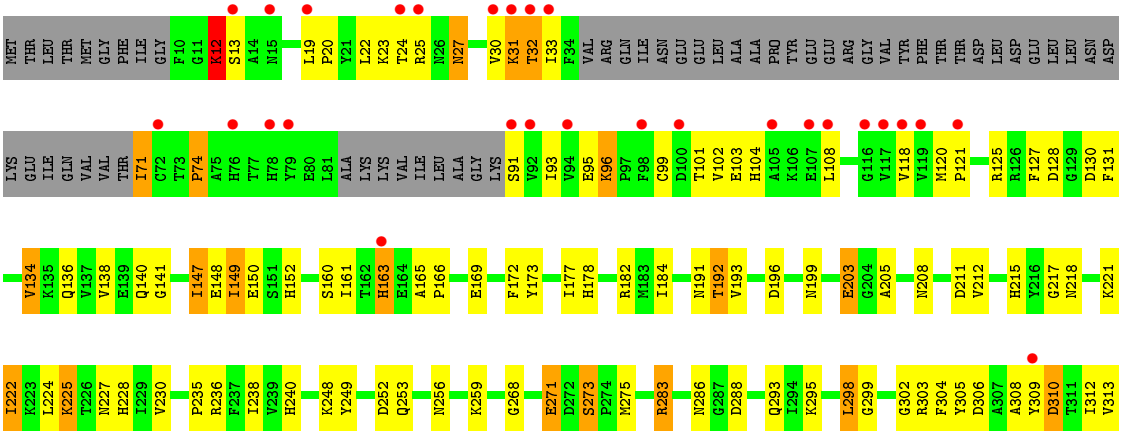
• Molecule 1: Oxidoreductase

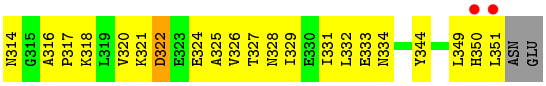
Chain D:



• Molecule 1: Oxidoreductase

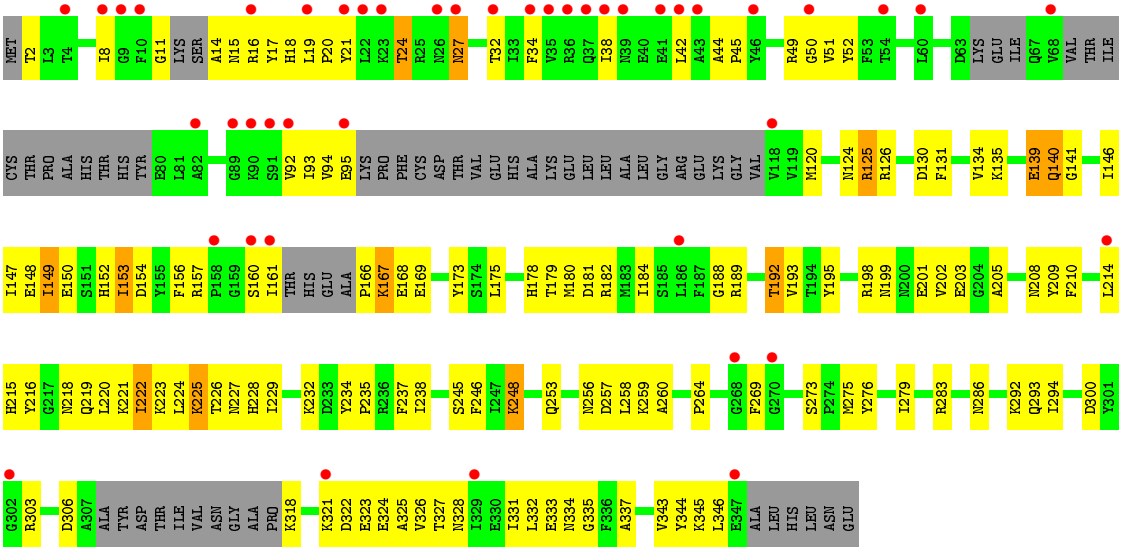
Chain E:





- Molecule 1: Oxidoreductase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.66Å 149.51Å 95.77Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	43.79 – 2.60 43.79 – 2.58	Depositor EDS
% Data completeness (in resolution range)	94.5 (43.79-2.60) 96.6 (43.79-2.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.59 (at 2.58Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.239 , 0.282 0.245 , 0.288	Depositor DCC
R_{free} test set	2966 reflections (4.00%)	DCC
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.4	EDS
Estimated twinning fraction	0.000 for l,k,-h 0.016 for h,-k,-l 0.012 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 157402 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15535	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.47	0/2831	0.69	0/3833
1	B	0.41	0/2841	0.64	0/3846
1	C	0.39	0/2728	0.62	0/3694
1	D	0.38	0/2793	0.60	0/3780
1	E	0.41	0/2352	0.64	1/3187 (0.0%)
1	F	0.35	0/2247	0.56	1/3038 (0.0%)
All	All	0.40	0/15792	0.63	2/21378 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	74	PRO	N-CA-CB	5.61	110.03	103.30
1	F	45	PRO	N-CA-CB	5.30	109.66	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2767	0	2702	110	0
1	B	2777	0	2721	126	0
1	C	2667	0	2578	112	0
1	D	2731	0	2674	146	0
1	E	2299	0	2150	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2205	0	1996	122	0
2	A	41	0	0	2	0
2	B	12	0	0	0	0
2	C	6	0	0	0	0
2	D	10	0	0	0	0
2	E	17	0	0	1	0
2	F	3	0	0	0	0
All	All	15535	0	14821	677	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 22.

All (677) 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:F:235:PRO:HG2	1:F:238:ILE:HD11	1.45	0.97
1:C:35:VAL:O	1:C:55:THR:HG22	1.65	0.95
1:B:191:ASN:HD21	1:B:217:GLY:H	1.10	0.93
1:B:26:ASN:ND2	1:B:26:ASN:H	1.67	0.91
1:D:110:ALA:HA	1:D:113:ARG:HD2	1.53	0.90
1:F:321:LYS:HB2	1:F:324:GLU:HG3	1.53	0.89
1:B:191:ASN:ND2	1:B:217:GLY:H	1.69	0.88
1:A:46:TYR:HB3	1:A:51:VAL:HG11	1.55	0.88
1:B:26:ASN:H	1:B:26:ASN:HD22	0.90	0.87
1:C:153:ILE:HD11	1:C:179:THR:HG23	1.55	0.86
1:B:26:ASN:HD22	1:B:26:ASN:N	1.72	0.86
1:B:46:TYR:HB3	1:B:51:VAL:HG11	1.59	0.85
1:A:23:LYS:HD3	1:A:49:ARG:NH1	1.92	0.85
1:F:120:MET:HB3	1:F:318:LYS:HD2	1.59	0.85
1:E:253:GLN:HE22	1:E:256:ASN:HD22	1.25	0.84
1:A:191:ASN:ND2	1:A:217:GLY:H	1.74	0.84
1:A:214:LEU:HB2	1:A:222:ILE:HG23	1.59	0.84
1:A:292:LYS:NZ	1:D:253:GLN:HE21	1.78	0.82
1:E:165:ALA:HB1	1:E:166:PRO:HD2	1.60	0.82
1:C:216:TYR:HB2	1:C:220:LEU:HB3	1.59	0.82
1:B:153:ILE:HD11	1:B:179:THR:HG21	1.63	0.81
1:E:192:THR:HG23	1:E:215:HIS:HB2	1.62	0.80
1:B:309:TYR:O	1:B:313:VAL:HG12	1.82	0.80
1:C:3:LEU:HD23	1:C:28:ILE:HD12	1.65	0.79
1:A:46:TYR:O	1:A:51:VAL:HG12	1.83	0.79
1:C:12:LYS:HE3	1:C:12:LYS:H	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ALA:HB3	1:B:45:PRO:HD3	1.64	0.77
1:B:46:TYR:O	1:B:51:VAL:HG12	1.84	0.76
1:C:149:ILE:HG22	1:C:222:ILE:HB	1.67	0.76
1:E:31:LYS:O	1:E:32:THR:CB	2.34	0.75
1:D:46:TYR:HB3	1:D:51:VAL:HG11	1.67	0.75
1:B:183:MET:HG3	1:B:222:ILE:HD13	1.68	0.75
1:D:313:VAL:HG13	1:D:314:ASN:H	1.50	0.75
1:B:12:LYS:HG2	1:B:13:SER:H	1.52	0.74
1:A:29:LYS:HE2	1:A:31:LYS:NZ	2.01	0.74
1:F:189:ARG:NH1	1:F:327:THR:HG23	2.03	0.74
1:A:183:MET:HG3	1:A:222:ILE:HD11	1.69	0.74
1:E:12:LYS:H	1:E:12:LYS:HD3	1.53	0.74
1:D:177:ILE:HD13	1:D:177:ILE:O	1.87	0.73
1:A:191:ASN:HD22	1:A:217:GLY:H	1.33	0.73
1:B:166:PRO:HG2	1:B:169:GLU:HG3	1.70	0.73
1:E:316:ALA:HB1	1:E:317:PRO:HD2	1.68	0.73
1:B:165:ALA:HB1	1:B:166:PRO:HD2	1.68	0.73
1:C:43:ALA:O	1:C:47:GLU:HG3	1.88	0.73
1:D:69:VAL:HG12	1:D:85:VAL:HG21	1.71	0.72
1:D:310:ASP:HB3	1:D:316:ALA:HB3	1.70	0.72
1:E:136:GLN:O	1:E:140:GLN:HG3	1.89	0.72
1:B:149:ILE:HG12	1:B:239:VAL:HG13	1.72	0.72
1:F:131:PHE:CE1	1:F:182:ARG:HB2	2.25	0.71
1:F:149:ILE:HD12	1:F:150:GLU:N	2.05	0.71
1:A:135:LYS:HG3	1:A:186:LEU:HD11	1.72	0.71
1:D:147:ILE:HD11	1:D:242:THR:HG23	1.72	0.71
1:B:189:ARG:HH22	1:B:330:GLU:CD	1.94	0.71
1:E:253:GLN:NE2	1:E:256:ASN:HD22	1.89	0.71
1:F:149:ILE:HA	1:F:238:ILE:O	1.91	0.70
1:C:46:TYR:HB3	1:C:51:VAL:HG11	1.73	0.70
1:A:211:ASP:CG	1:A:225:LYS:HD3	2.12	0.70
1:B:81:LEU:O	1:B:85:VAL:HG12	1.91	0.70
1:C:49:ARG:HA	1:C:49:ARG:NE	2.07	0.70
1:F:166:PRO:HD2	1:F:169:GLU:HG3	1.72	0.69
1:D:4:THR:HG23	1:D:31:LYS:HG2	1.73	0.69
1:D:46:TYR:O	1:D:51:VAL:HG12	1.92	0.69
1:F:220:LEU:HD12	1:F:221:LYS:H	1.55	0.69
1:F:2:THR:HG22	1:F:27:ASN:ND2	2.07	0.69
1:E:193:VAL:HG21	1:E:331:ILE:HD12	1.73	0.69
1:C:82:ALA:O	1:C:86:ILE:HG13	1.92	0.69
1:A:165:ALA:HB1	1:A:166:PRO:HD2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:MET:HB3	1:E:318:LYS:HD2	1.74	0.69
1:B:199:ASN:HA	1:B:208:ASN:OD1	1.93	0.69
1:F:220:LEU:HD12	1:F:221:LYS:N	2.08	0.69
1:E:322:ASP:O	1:E:326:VAL:HG12	1.93	0.69
1:B:192:THR:HG23	1:B:215:HIS:HB2	1.75	0.68
1:E:150:GLU:OE2	1:E:152:HIS:HE1	1.76	0.68
1:D:309:TYR:O	1:D:313:VAL:HG12	1.94	0.68
1:A:66:ILE:HB	1:A:90:LYS:NZ	2.07	0.68
1:F:189:ARG:HH11	1:F:327:THR:HG23	1.57	0.67
1:A:29:LYS:HE2	1:A:31:LYS:HZ2	1.59	0.67
1:D:221:LYS:HD2	1:F:198:ARG:HH21	1.57	0.67
1:C:309:TYR:O	1:C:313:VAL:HG12	1.94	0.67
1:A:57:LEU:HG	1:A:61:LEU:HD23	1.77	0.67
1:C:149:ILE:HG12	1:C:239:VAL:HG22	1.76	0.67
1:B:109:LEU:HD22	1:B:322:ASP:OD1	1.95	0.67
1:B:25:ARG:NH2	1:B:302:GLY:HA3	2.10	0.67
1:A:69:VAL:CG1	1:A:85:VAL:HG21	2.24	0.67
1:B:69:VAL:HG13	1:B:85:VAL:HG21	1.78	0.66
1:D:120:MET:HB3	1:D:318:LYS:HD2	1.76	0.66
1:F:228:HIS:O	1:F:229:ILE:HD13	1.96	0.66
1:B:160:SER:HB3	1:B:161:ILE:HD12	1.76	0.66
1:A:225:LYS:HD2	2:A:369:HOH:O	1.94	0.66
1:F:253:GLN:NE2	1:F:256:ASN:HD22	1.93	0.66
1:C:99:CYS:SG	1:C:108:LEU:HD22	2.36	0.66
1:C:327:THR:O	1:C:331:ILE:HG12	1.96	0.66
1:B:211:ASP:CG	1:B:225:LYS:HD3	2.17	0.65
1:F:293:GLN:C	1:F:294:ILE:HD12	2.16	0.65
1:E:19:LEU:HB2	1:E:20:PRO:HD3	1.77	0.65
1:E:313:VAL:HG13	1:E:314:ASN:OD1	1.97	0.65
1:B:113:ARG:HH11	1:B:113:ARG:HB3	1.62	0.65
1:E:27:ASN:N	1:E:27:ASN:HD22	1.95	0.65
1:E:12:LYS:HG2	1:E:13:SER:H	1.62	0.64
1:E:306:ASP:O	1:E:310:ASP:HB2	1.97	0.64
1:E:12:LYS:H	1:E:12:LYS:CD	2.09	0.64
1:F:19:LEU:HB2	1:F:20:PRO:HD3	1.79	0.64
1:C:229:ILE:N	1:C:229:ILE:HD12	2.12	0.64
1:D:123:GLN:HE22	1:D:177:ILE:HD11	1.63	0.64
1:F:94:VAL:HG12	1:F:95:GLU:H	1.61	0.64
1:D:149:ILE:HB	1:D:222:ILE:HG22	1.78	0.64
1:E:199:ASN:HA	1:E:208:ASN:OD1	1.98	0.64
1:D:198:ARG:HB2	1:F:218:ASN:HD21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLU:OE2	1:C:152:HIS:HE1	1.81	0.64
1:B:12:LYS:H	1:B:12:LYS:HD2	1.64	0.64
1:C:75:ALA:HB1	1:C:97:PRO:HD2	1.80	0.64
1:C:192:THR:HG23	1:C:215:HIS:HB2	1.79	0.63
1:A:7:PHE:HB2	1:A:33:ILE:HD13	1.80	0.63
1:F:21:TYR:O	1:F:24:THR:HG22	1.98	0.63
1:F:149:ILE:HG13	1:F:222:ILE:HD13	1.81	0.63
1:A:81:LEU:O	1:A:85:VAL:HG12	1.98	0.63
1:F:166:PRO:HG2	1:F:169:GLU:HG2	1.79	0.63
1:E:253:GLN:HE21	1:F:292:LYS:NZ	1.97	0.63
1:C:17:TYR:OH	1:C:255:GLU:HG3	1.99	0.63
1:C:19:LEU:HB2	1:C:20:PRO:HD3	1.79	0.63
1:A:147:ILE:HG13	1:A:148:GLU:N	2.13	0.63
1:C:35:VAL:O	1:C:55:THR:CG2	2.42	0.62
1:A:150:GLU:OE2	1:A:152:HIS:HE1	1.83	0.62
1:D:96:LYS:HB3	1:D:96:LYS:NZ	2.14	0.62
1:E:222:ILE:HD11	1:E:224:LEU:HD21	1.81	0.62
1:D:172:PHE:CE1	1:D:212:VAL:HG21	2.34	0.62
1:A:44:ALA:HB3	1:A:45:PRO:HD3	1.81	0.62
1:C:69:VAL:HG12	1:C:85:VAL:HG21	1.80	0.62
1:B:12:LYS:HG2	1:B:13:SER:N	2.14	0.62
1:D:109:LEU:HD11	1:D:322:ASP:HB3	1.81	0.62
1:A:96:LYS:HD2	1:A:177:ILE:HG21	1.82	0.62
1:D:166:PRO:HB2	1:D:168:GLU:OE1	1.99	0.62
1:F:210:PHE:CE2	1:F:226:THR:HB	2.35	0.62
1:D:313:VAL:HG13	1:D:314:ASN:N	2.14	0.62
1:C:101:THR:HB	1:C:103:GLU:OE2	2.00	0.61
1:C:73:THR:HB	1:C:74:PRO:HD2	1.81	0.61
1:C:83:LYS:HA	1:C:86:ILE:HD12	1.82	0.61
1:D:192:THR:HG23	1:D:215:HIS:HB2	1.82	0.61
1:A:12:LYS:N	1:A:12:LYS:HD2	2.15	0.61
1:B:219:GLN:HG2	1:C:200:ASN:O	2.00	0.61
1:C:209:TYR:CD1	1:C:210:PHE:N	2.69	0.61
1:C:126:ARG:NH2	1:C:324:GLU:OE1	2.28	0.61
1:B:293:GLN:HB2	1:F:273:SER:HB3	1.81	0.60
1:C:165:ALA:HB1	1:C:166:PRO:HD2	1.83	0.60
1:E:134:VAL:O	1:E:138:VAL:HG23	2.02	0.60
1:A:23:LYS:HD3	1:A:49:ARG:CZ	2.31	0.60
1:A:210:PHE:CE2	1:A:226:THR:HB	2.36	0.60
1:D:25:ARG:HH12	1:D:302:GLY:HA3	1.66	0.60
1:C:153:ILE:CD1	1:C:179:THR:HG23	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:H	1:A:12:LYS:HZ3	1.50	0.60
1:C:125:ARG:HG3	1:C:178:HIS:CG	2.37	0.60
1:D:214:LEU:HD12	1:D:222:ILE:HD11	1.82	0.60
1:C:73:THR:HB	1:C:74:PRO:CD	2.31	0.60
1:A:125:ARG:HB2	2:A:361:HOH:O	2.02	0.60
1:B:46:TYR:O	1:B:51:VAL:CG1	2.50	0.59
1:F:199:ASN:OD1	1:F:201:GLU:HB2	2.01	0.59
1:F:146:ILE:H	1:F:146:ILE:HD12	1.66	0.59
1:F:146:ILE:N	1:F:146:ILE:HD12	2.17	0.59
1:E:235:PRO:HG3	1:E:249:TYR:CZ	2.37	0.59
1:B:63:ASP:HB3	1:B:66:ILE:HD13	1.85	0.59
1:A:66:ILE:HB	1:A:90:LYS:HZ1	1.67	0.59
1:A:262:ILE:HG22	1:A:266:SER:OG	2.03	0.59
1:B:26:ASN:ND2	1:B:26:ASN:N	2.38	0.59
1:A:344:TYR:HE2	1:A:346:LEU:HD13	1.68	0.59
1:E:22:LEU:HD21	1:E:305:TYR:CD2	2.38	0.59
1:C:199:ASN:HA	1:C:208:ASN:OD1	2.03	0.59
1:A:214:LEU:HB2	1:A:222:ILE:CG2	2.31	0.58
1:A:75:ALA:HB1	1:A:97:PRO:HD2	1.84	0.58
1:B:131:PHE:CD1	1:B:182:ARG:HD2	2.38	0.58
1:A:96:LYS:HE3	1:A:174:SER:HA	1.85	0.58
1:C:6:GLY:C	1:C:69:VAL:HG23	2.23	0.58
1:C:83:LYS:O	1:C:87:LEU:HD13	2.04	0.58
1:F:248:LYS:HE3	1:F:276:TYR:O	2.04	0.58
1:E:268:GLY:HA2	1:E:271:GLU:HG3	1.86	0.58
1:F:16:ARG:NH1	1:F:259:LYS:HG2	2.19	0.58
1:A:240:HIS:CE1	1:E:230:VAL:HG13	2.38	0.58
1:B:281:LYS:HA	1:B:290:ILE:O	2.04	0.58
1:B:161:ILE:N	1:B:161:ILE:HD12	2.19	0.58
1:D:157:ARG:O	1:D:160:SER:HB2	2.02	0.57
1:B:25:ARG:HH21	1:B:302:GLY:HA3	1.69	0.57
1:B:211:ASP:OD2	1:B:225:LYS:HD3	2.04	0.57
1:D:73:THR:OG1	1:D:74:PRO:HD2	2.05	0.57
1:A:199:ASN:HA	1:A:208:ASN:OD1	2.04	0.57
1:A:69:VAL:HG12	1:A:85:VAL:HG21	1.85	0.57
1:D:131:PHE:CE1	1:D:182:ARG:HB2	2.40	0.57
1:D:235:PRO:HG3	1:D:249:TYR:CZ	2.38	0.57
1:E:173:TYR:CD2	1:E:332:LEU:HD23	2.39	0.57
1:F:32:THR:HA	1:F:52:TYR:O	2.04	0.57
1:A:211:ASP:OD2	1:A:225:LYS:HD3	2.04	0.57
1:E:222:ILE:HD13	1:E:222:ILE:C	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:HIS:ND1	1:D:305:TYR:OH	2.31	0.57
1:A:7:PHE:HB2	1:A:33:ILE:CD1	2.34	0.57
1:B:150:GLU:OE2	1:B:152:HIS:HE1	1.87	0.57
1:F:222:ILE:HD12	1:F:223:LYS:N	2.20	0.56
1:B:191:ASN:HD21	1:B:217:GLY:N	1.91	0.56
1:D:146:ILE:HG22	1:D:220:LEU:HD13	1.86	0.56
1:D:145:ASP:O	1:D:147:ILE:HD12	2.04	0.56
1:B:113:ARG:HB3	1:B:113:ARG:NH1	2.21	0.56
1:C:86:ILE:HG12	1:C:92:VAL:HG21	1.88	0.56
1:E:222:ILE:HD13	1:E:222:ILE:O	2.05	0.56
1:F:328:ASN:O	1:F:332:LEU:HD23	2.04	0.56
1:C:253:GLN:HE22	1:C:256:ASN:HD22	1.54	0.56
1:C:313:VAL:HG13	1:C:314:ASN:ND2	2.21	0.56
1:F:303:ARG:HA	1:F:306:ASP:OD2	2.06	0.56
1:E:236:ARG:N	1:E:248:LYS:O	2.39	0.56
1:C:135:LYS:HG3	1:C:186:LEU:HD11	1.88	0.56
1:B:135:LYS:HG3	1:B:186:LEU:HD11	1.87	0.56
1:E:191:ASN:HD22	1:E:217:GLY:H	1.52	0.56
1:B:153:ILE:CD1	1:B:179:THR:HG21	2.36	0.55
1:F:161:ILE:N	1:F:161:ILE:HD12	2.21	0.55
1:C:283:ARG:HG3	1:C:283:ARG:HH11	1.71	0.55
1:D:99:CYS:SG	1:D:108:LEU:HD12	2.46	0.55
1:C:44:ALA:HB3	1:C:45:PRO:HD3	1.87	0.55
1:D:183:MET:HB3	1:D:222:ILE:HD12	1.88	0.55
1:E:321:LYS:HB2	1:E:324:GLU:HG3	1.88	0.55
1:B:82:ALA:HB3	1:B:108:LEU:HD21	1.88	0.55
1:D:5:MET:HE3	1:D:28:ILE:HG21	1.88	0.55
1:E:30:VAL:O	1:E:31:LYS:CB	2.55	0.55
1:F:147:ILE:HG22	1:F:219:GLN:HG2	1.89	0.55
1:A:69:VAL:HG11	1:A:85:VAL:HG21	1.89	0.55
1:C:193:VAL:HG21	1:C:331:ILE:HD12	1.89	0.54
1:C:209:TYR:CD1	1:C:209:TYR:C	2.80	0.54
1:C:277:TYR:OH	1:C:295:LYS:HE3	2.08	0.54
1:B:73:THR:HB	1:B:74:PRO:CD	2.37	0.54
1:B:125:ARG:NH1	1:B:128:ASP:OD2	2.40	0.54
1:D:184:ILE:HD12	1:D:328:ASN:OD1	2.07	0.54
1:B:280:ALA:O	1:B:291:GLU:HA	2.07	0.54
1:B:259:LYS:HZ2	1:E:286:ASN:ND2	2.06	0.54
1:C:134:VAL:O	1:C:138:VAL:HG23	2.08	0.54
1:F:184:ILE:HG23	1:F:188:GLY:O	2.08	0.54
1:E:298:LEU:HD23	1:E:299:GLY:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD22	1:B:28:ILE:HG21	1.90	0.54
1:A:293:GLN:HB2	1:D:273:SER:HB2	1.90	0.54
1:F:157:ARG:HB3	1:F:160:SER:HB2	1.90	0.53
1:C:321:LYS:O	1:C:324:GLU:HB2	2.07	0.53
1:C:172:PHE:CE1	1:C:212:VAL:HG21	2.43	0.53
1:F:294:ILE:HD12	1:F:294:ILE:N	2.22	0.53
1:E:125:ARG:HD2	1:E:178:HIS:CG	2.43	0.53
1:B:274:PRO:HD2	1:E:293:GLN:OE1	2.08	0.53
1:A:111:LEU:O	1:A:115:LYS:HB2	2.09	0.53
1:D:165:ALA:HB1	1:D:166:PRO:HD2	1.89	0.53
1:D:5:MET:CE	1:D:28:ILE:HG21	2.39	0.53
1:A:109:LEU:HD22	1:A:322:ASP:OD1	2.08	0.53
1:C:149:ILE:CG2	1:C:222:ILE:HB	2.37	0.53
1:D:60:LEU:O	1:D:63:ASP:HB2	2.09	0.53
1:F:201:GLU:HG2	1:F:208:ASN:HD21	1.74	0.53
1:B:161:ILE:H	1:B:161:ILE:HD12	1.74	0.53
1:A:29:LYS:HE2	1:A:31:LYS:HZ1	1.74	0.53
1:D:4:THR:HG23	1:D:31:LYS:CG	2.39	0.53
1:C:144:GLY:O	1:C:146:ILE:HD12	2.09	0.53
1:F:131:PHE:HA	1:F:134:VAL:HG22	1.91	0.52
1:F:202:VAL:HG23	1:F:205:ALA:CB	2.39	0.52
1:F:343:VAL:HG12	1:F:344:TYR:N	2.24	0.52
1:C:46:TYR:HB3	1:C:51:VAL:CG1	2.39	0.52
1:A:57:LEU:HG	1:A:61:LEU:CD2	2.39	0.52
1:F:209:TYR:O	1:F:210:PHE:HB3	2.08	0.52
1:F:175:LEU:O	1:F:178:HIS:HB2	2.09	0.52
1:D:321:LYS:HB2	1:D:324:GLU:HG3	1.91	0.52
1:D:150:GLU:OE2	1:D:152:HIS:HE1	1.91	0.52
1:C:326:VAL:HG13	1:C:327:THR:N	2.24	0.52
1:B:138:VAL:HG22	1:B:146:ILE:CD1	2.39	0.52
1:C:35:VAL:CG1	1:C:38:ILE:HG12	2.39	0.52
1:F:92:VAL:HG12	1:F:93:ILE:N	2.24	0.52
1:A:135:LYS:HG3	1:A:186:LEU:CD1	2.40	0.52
1:A:283:ARG:HA	1:A:288:ASP:O	2.09	0.52
1:A:121:PRO:HG2	1:A:320:VAL:HG11	1.91	0.52
1:E:131:PHE:CE1	1:E:182:ARG:HB2	2.44	0.52
1:A:29:LYS:HB3	1:A:31:LYS:NZ	2.24	0.52
1:E:22:LEU:C	1:E:24:THR:H	2.13	0.52
1:D:21:TYR:CZ	1:D:301:TYR:HB2	2.44	0.52
1:B:73:THR:HB	1:B:74:PRO:HD2	1.92	0.52
1:E:102:VAL:HG13	1:E:103:GLU:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ALA:HB1	1:C:97:PRO:CD	2.40	0.52
1:C:214:LEU:HG	1:C:222:ILE:HD11	1.92	0.51
1:D:147:ILE:N	1:D:147:ILE:HD12	2.26	0.51
1:D:199:ASN:O	1:D:201:GLU:N	2.43	0.51
1:D:281:LYS:HA	1:D:290:ILE:O	2.10	0.51
1:A:292:LYS:HZ2	1:D:253:GLN:HE21	1.56	0.51
1:D:25:ARG:HH12	1:D:302:GLY:CA	2.22	0.51
1:D:128:ASP:HB3	1:D:130:ASP:OD2	2.10	0.51
1:C:268:GLY:HA2	1:C:271:GLU:OE1	2.11	0.51
1:B:286:ASN:ND2	1:F:259:LYS:NZ	2.59	0.51
1:B:259:LYS:NZ	1:E:286:ASN:ND2	2.59	0.51
1:B:259:LYS:NZ	1:E:286:ASN:HD21	2.09	0.51
1:A:113:ARG:HB3	1:A:113:ARG:NH1	2.25	0.51
1:D:110:ALA:CA	1:D:113:ARG:HD2	2.35	0.51
1:A:46:TYR:C	1:A:51:VAL:HG12	2.30	0.51
1:C:106:LYS:HB2	1:C:106:LYS:NZ	2.26	0.51
1:B:102:VAL:HG13	1:B:103:GLU:OE2	2.10	0.51
1:B:102:VAL:O	1:B:106:LYS:HG3	2.10	0.51
1:D:82:ALA:O	1:D:86:ILE:HG12	2.11	0.51
1:E:160:SER:HB3	1:E:161:ILE:HD12	1.92	0.51
1:D:61:LEU:H	1:D:61:LEU:HD22	1.74	0.51
1:A:60:LEU:C	1:A:60:LEU:HD23	2.31	0.51
1:D:196:ASP:HA	1:D:340:SER:OG	2.11	0.51
1:B:47:GLU:C	1:B:49:ARG:H	2.14	0.51
1:C:46:TYR:O	1:C:51:VAL:HG12	2.11	0.51
1:A:43:ALA:O	1:A:47:GLU:HG3	2.11	0.50
1:D:161:ILE:N	1:D:161:ILE:HD12	2.26	0.50
1:C:8:ILE:HG13	1:C:69:VAL:HG21	1.94	0.50
1:F:192:THR:HA	1:F:346:LEU:HD23	1.93	0.50
1:B:149:ILE:CG1	1:B:239:VAL:HG13	2.41	0.50
1:B:27:ASN:HB3	1:B:309:TYR:CE1	2.47	0.50
1:A:196:ASP:O	1:A:210:PHE:HA	2.11	0.50
1:F:167:LYS:HB2	1:F:173:TYR:CZ	2.46	0.50
1:F:134:VAL:HG11	1:F:237:PHE:CB	2.41	0.50
1:F:323:GLU:HA	1:F:326:VAL:HG12	1.93	0.50
1:B:263:MET:HB2	1:B:265:GLU:OE2	2.12	0.50
1:D:253:GLN:HE22	1:D:256:ASN:HD22	1.60	0.50
1:E:309:TYR:CZ	1:E:313:VAL:HG11	2.45	0.50
1:B:7:PHE:HB2	1:B:33:ILE:HG12	1.94	0.50
1:B:322:ASP:O	1:B:326:VAL:HG12	2.11	0.50
1:A:12:LYS:NZ	1:A:12:LYS:H	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:H	1:A:12:LYS:HD2	1.77	0.50
1:B:131:PHE:CE1	1:B:182:ARG:HB2	2.47	0.50
1:A:75:ALA:CB	1:A:97:PRO:HD2	2.41	0.50
1:E:298:LEU:HD23	1:E:299:GLY:N	2.27	0.50
1:B:138:VAL:HG22	1:B:146:ILE:HD11	1.93	0.50
1:D:198:ARG:HH21	1:F:221:LYS:HD2	1.77	0.49
1:C:184:ILE:HG23	1:C:188:GLY:O	2.12	0.49
1:E:71:ILE:HD12	1:E:71:ILE:N	2.27	0.49
1:D:210:PHE:O	1:D:210:PHE:CD1	2.65	0.49
1:F:202:VAL:HG23	1:F:205:ALA:HB2	1.93	0.49
1:F:150:GLU:OE2	1:F:152:HIS:HE1	1.95	0.49
1:B:49:ARG:O	1:B:51:VAL:N	2.45	0.49
1:B:196:ASP:HB3	1:B:211:ASP:HB3	1.94	0.49
1:C:149:ILE:CG1	1:C:239:VAL:HG22	2.39	0.49
1:C:94:VAL:HB	1:C:98:PHE:HD1	1.76	0.49
1:D:69:VAL:CG1	1:D:85:VAL:HG21	2.42	0.49
1:F:345:LYS:C	1:F:346:LEU:HD22	2.33	0.49
1:B:19:LEU:HB2	1:B:20:PRO:HD3	1.94	0.49
1:D:221:LYS:HD2	1:F:198:ARG:NH2	2.25	0.49
1:E:275:MET:HB2	1:F:293:GLN:CD	2.33	0.49
1:A:147:ILE:HD12	1:E:227:ASN:HD21	1.78	0.49
1:E:102:VAL:HG13	1:E:103:GLU:H	1.78	0.49
1:B:143:LEU:C	1:B:243:ASN:HB2	2.33	0.49
1:B:172:PHE:CE1	1:B:212:VAL:HG21	2.47	0.49
1:A:203:GLU:OE2	1:E:218:ASN:HB2	2.13	0.49
1:F:153:ILE:HD12	1:F:179:THR:HG23	1.95	0.49
1:E:273:SER:HB3	1:F:293:GLN:HB2	1.94	0.49
1:A:125:ARG:HG3	1:A:178:HIS:CG	2.47	0.49
1:E:104:HIS:O	1:E:108:LEU:HB2	2.12	0.49
1:D:136:GLN:O	1:D:140:GLN:HG3	2.12	0.49
1:B:293:GLN:HG3	1:F:275:MET:HE2	1.94	0.49
1:D:149:ILE:HD12	1:D:187:PHE:CE2	2.48	0.49
1:F:146:ILE:CD1	1:F:146:ILE:H	2.26	0.49
1:C:149:ILE:HG22	1:C:222:ILE:CB	2.39	0.48
1:F:161:ILE:CD1	1:F:208:ASN:HD22	2.26	0.48
1:D:211:ASP:OD2	1:D:225:LYS:HD3	2.12	0.48
1:D:58:ASP:HB3	1:D:62:ASN:ND2	2.28	0.48
1:D:199:ASN:HA	1:D:208:ASN:OD1	2.12	0.48
1:E:149:ILE:HA	1:E:238:ILE:O	2.14	0.48
1:A:82:ALA:O	1:A:86:ILE:HG13	2.13	0.48
1:C:111:LEU:O	1:C:115:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LYS:HD2	1:D:174:SER:HA	1.95	0.48
1:C:322:ASP:O	1:C:326:VAL:HG12	2.13	0.48
1:E:308:ALA:O	1:E:312:ILE:HD13	2.14	0.48
1:B:171:SER:OG	1:B:208:ASN:HA	2.13	0.48
1:C:253:GLN:HA	1:C:253:GLN:HE21	1.77	0.48
1:F:192:THR:HG23	1:F:215:HIS:HB2	1.95	0.48
1:E:125:ARG:C	1:E:127:PHE:H	2.17	0.48
1:C:146:ILE:N	1:C:146:ILE:HD12	2.28	0.48
1:F:153:ILE:CD1	1:F:179:THR:HG23	2.44	0.48
1:A:25:ARG:HD2	1:A:306:ASP:OD1	2.13	0.48
1:D:135:LYS:O	1:D:139:GLU:HG3	2.13	0.48
1:E:211:ASP:OD2	1:E:225:LYS:HD3	2.14	0.48
1:E:259:LYS:NZ	1:F:286:ASN:ND2	2.61	0.48
1:B:223:LYS:NZ	1:C:223:LYS:NZ	2.62	0.48
1:C:3:LEU:HB3	1:C:28:ILE:HD13	1.95	0.48
1:E:148:GLU:HA	1:E:221:LYS:O	2.13	0.48
1:D:73:THR:HG21	1:D:81:LEU:CD1	2.44	0.48
1:D:131:PHE:CD1	1:D:182:ARG:HD2	2.48	0.48
1:D:231:ALA:HB3	1:F:245:SER:OG	2.14	0.48
1:E:334:ASN:ND2	1:E:344:TYR:CE1	2.82	0.48
1:D:31:LYS:HB2	1:D:66:ILE:HD11	1.94	0.48
1:D:40:GLU:HA	1:D:43:ALA:HB3	1.95	0.48
1:E:27:ASN:N	1:E:27:ASN:ND2	2.60	0.48
1:F:180:MET:HB2	1:F:224:LEU:HD13	1.96	0.48
1:B:283:ARG:HA	1:B:288:ASP:O	2.14	0.48
1:E:150:GLU:OE2	1:E:152:HIS:CE1	2.61	0.47
1:C:283:ARG:HA	1:C:288:ASP:O	2.14	0.47
1:B:102:VAL:HG12	1:B:333:GLU:OE2	2.13	0.47
1:E:172:PHE:CZ	1:E:212:VAL:HG21	2.49	0.47
1:F:321:LYS:HB2	1:F:324:GLU:CG	2.33	0.47
1:D:39:ASN:ND2	1:D:42:LEU:H	2.12	0.47
1:D:39:ASN:HD21	1:D:41:GLU:HB3	1.79	0.47
1:D:46:TYR:O	1:D:51:VAL:CG1	2.60	0.47
1:D:96:LYS:HZ2	1:D:96:LYS:HB3	1.77	0.47
1:E:327:THR:O	1:E:331:ILE:HG12	2.14	0.47
1:E:283:ARG:HA	1:E:288:ASP:O	2.14	0.47
1:B:136:GLN:O	1:B:140:GLN:HG3	2.13	0.47
1:A:122:TYR:CZ	1:A:124:ASN:HB3	2.50	0.47
1:F:214:LEU:HB2	1:F:222:ILE:HG23	1.96	0.47
1:C:193:VAL:HG21	1:C:331:ILE:HG23	1.95	0.47
1:A:240:HIS:ND1	1:A:245:SER:HB3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:SER:HB2	1:F:293:GLN:OE1	2.15	0.47
1:D:179:THR:HG22	1:D:182:ARG:HH21	1.80	0.47
1:C:131:PHE:CE1	1:C:182:ARG:HB2	2.49	0.47
1:B:235:PRO:HG3	1:B:249:TYR:CZ	2.49	0.47
1:C:71:ILE:N	1:C:71:ILE:HD12	2.29	0.47
1:A:292:LYS:HZ1	1:D:253:GLN:HE21	1.56	0.47
1:F:94:VAL:HG12	1:F:95:GLU:N	2.29	0.47
1:A:147:ILE:O	1:A:220:LEU:HA	2.15	0.47
1:D:195:TYR:CE2	1:D:335:GLY:HA2	2.49	0.47
1:C:153:ILE:HD11	1:C:179:THR:CG2	2.36	0.47
1:B:25:ARG:NH1	1:B:306:ASP:OD2	2.47	0.47
1:A:109:LEU:O	1:A:113:ARG:HG3	2.14	0.47
1:D:199:ASN:C	1:D:201:GLU:H	2.18	0.47
1:E:128:ASP:HA	1:E:252:ASP:OD2	2.14	0.47
1:D:283:ARG:HA	1:D:288:ASP:O	2.15	0.47
1:A:344:TYR:CE2	1:A:346:LEU:HD13	2.47	0.47
1:A:82:ALA:HB3	1:A:108:LEU:HD21	1.96	0.47
1:A:147:ILE:CD1	1:E:227:ASN:HD21	2.28	0.47
1:B:236:ARG:CZ	1:B:251:GLU:HB2	2.45	0.47
1:B:149:ILE:O	1:B:222:ILE:HA	2.15	0.47
1:D:111:LEU:O	1:D:111:LEU:HD23	2.15	0.47
1:F:134:VAL:HG11	1:F:237:PHE:CG	2.51	0.46
1:C:69:VAL:CG1	1:C:85:VAL:HG21	2.45	0.46
1:C:253:GLN:HA	1:C:253:GLN:NE2	2.30	0.46
1:D:86:ILE:O	1:D:115:LYS:HE2	2.15	0.46
1:A:23:LYS:HA	1:A:23:LYS:HE2	1.97	0.46
1:E:166:PRO:HG2	1:E:169:GLU:HG2	1.97	0.46
1:D:167:LYS:HG3	1:D:168:GLU:OE2	2.15	0.46
1:D:96:LYS:HD2	1:D:174:SER:O	2.15	0.46
1:F:131:PHE:CZ	1:F:182:ARG:HB2	2.50	0.46
1:D:214:LEU:O	1:D:216:TYR:HD2	1.97	0.46
1:F:209:TYR:CD1	1:F:210:PHE:N	2.83	0.46
1:F:343:VAL:HG12	1:F:344:TYR:H	1.80	0.46
1:B:78:HIS:CE1	1:B:95:GLU:O	2.68	0.46
1:D:325:ALA:O	1:D:329:ILE:HG12	2.15	0.46
1:B:133:ALA:HB2	1:B:297:PRO:HD2	1.97	0.46
1:F:140:GLN:HB3	1:F:140:GLN:HE21	1.58	0.46
1:E:328:ASN:O	1:E:332:LEU:HD13	2.16	0.46
1:A:167:LYS:HE3	1:A:168:GLU:OE2	2.16	0.46
1:F:11:GLY:C	1:F:15:ASN:H	2.18	0.46
1:D:110:ALA:O	1:D:113:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ALA:O	1:B:47:GLU:HG3	2.15	0.46
1:F:131:PHE:CD1	1:F:182:ARG:HD2	2.50	0.46
1:D:58:ASP:HB3	1:D:62:ASN:HD22	1.80	0.46
1:D:13:SER:HB3	1:D:95:GLU:OE2	2.16	0.46
1:E:177:ILE:HD11	1:E:328:ASN:HD22	1.80	0.46
1:A:229:ILE:HD12	1:A:229:ILE:N	2.30	0.46
1:F:234:TYR:HB3	1:F:235:PRO:CD	2.46	0.46
1:A:51:VAL:HG13	1:A:51:VAL:O	2.15	0.46
1:C:75:ALA:HA	1:C:78:HIS:CE1	2.50	0.46
1:F:181:ASP:CB	1:F:328:ASN:HD21	2.29	0.46
1:E:329:ILE:HD12	1:E:329:ILE:N	2.31	0.46
1:E:350:HIS:O	1:E:351:LEU:HD23	2.16	0.46
1:D:60:LEU:HD21	1:D:69:VAL:HG21	1.98	0.46
1:C:83:LYS:HB3	1:C:108:LEU:HD11	1.97	0.46
1:D:146:ILE:HD12	1:D:146:ILE:N	2.31	0.46
1:B:283:ARG:HG3	1:B:283:ARG:HH11	1.81	0.45
1:D:134:VAL:O	1:D:138:VAL:HG23	2.16	0.45
1:B:44:ALA:HB3	1:B:45:PRO:CD	2.42	0.45
1:E:273:SER:CB	1:F:293:GLN:HB2	2.46	0.45
1:B:131:PHE:CG	1:B:182:ARG:HD2	2.51	0.45
1:B:122:TYR:CZ	1:B:124:ASN:HB3	2.51	0.45
1:B:125:ARG:HD2	1:B:178:HIS:CG	2.51	0.45
1:A:209:TYR:CD1	1:A:210:PHE:N	2.84	0.45
1:D:198:ARG:NH2	1:F:221:LYS:HD2	2.32	0.45
1:D:303:ARG:HA	1:D:306:ASP:OD2	2.16	0.45
1:B:240:HIS:CE1	1:C:230:VAL:HG13	2.52	0.45
1:A:149:ILE:HA	1:A:238:ILE:O	2.17	0.45
1:E:275:MET:HB2	1:F:293:GLN:OE1	2.17	0.45
1:A:316:ALA:HB1	1:A:317:PRO:HD2	1.98	0.45
1:D:150:GLU:HB3	1:D:238:ILE:HB	1.99	0.45
1:E:325:ALA:O	1:E:329:ILE:HD13	2.17	0.45
1:A:83:LYS:O	1:A:87:LEU:HD22	2.17	0.45
1:F:199:ASN:OD1	1:F:202:VAL:N	2.49	0.45
1:C:306:ASP:O	1:C:309:TYR:HB3	2.17	0.45
1:B:16:ARG:HH12	1:B:259:LYS:HE2	1.82	0.45
1:D:91:SER:N	1:D:117:VAL:HB	2.31	0.45
1:A:192:THR:HG23	1:A:215:HIS:HB2	1.98	0.45
1:E:163:HIS:O	1:E:205:ALA:HB1	2.17	0.45
1:E:141:GLY:HA2	2:E:362:HOH:O	2.16	0.45
1:A:47:GLU:O	1:A:49:ARG:O	2.35	0.44
1:A:185:SER:HA	1:A:324:GLU:OE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:TYR:HB3	1:C:197:ILE:CD1	2.47	0.44
1:B:190:PRO:HB3	1:B:216:TYR:CE2	2.52	0.44
1:D:110:ALA:C	1:D:112:GLY:H	2.21	0.44
1:C:149:ILE:HD13	1:C:150:GLU:H	1.82	0.44
1:E:268:GLY:O	1:E:271:GLU:HB2	2.16	0.44
1:D:76:HIS:ND1	1:D:77:THR:HG23	2.32	0.44
1:B:148:GLU:HA	1:B:221:LYS:O	2.17	0.44
1:F:227:ASN:OD1	1:F:229:ILE:N	2.38	0.44
1:F:11:GLY:HA2	1:F:15:ASN:HD22	1.81	0.44
1:A:274:PRO:HA	1:A:277:TYR:CE1	2.52	0.44
1:F:135:LYS:HG2	1:F:139:GLU:OE1	2.17	0.44
1:E:165:ALA:HB1	1:E:166:PRO:CD	2.41	0.44
1:D:96:LYS:HG3	1:D:177:ILE:HG21	1.98	0.44
1:A:71:ILE:HD13	1:A:81:LEU:HB2	1.99	0.44
1:F:131:PHE:CG	1:F:182:ARG:HD2	2.53	0.44
1:E:326:VAL:HG13	1:E:349:LEU:HD11	2.00	0.44
1:D:89:GLY:C	1:D:117:VAL:HG11	2.37	0.44
1:D:247:ILE:HD13	1:F:232:LYS:HG2	2.00	0.44
1:C:264:PRO:HA	1:C:269:PHE:CD2	2.52	0.44
1:F:14:ALA:O	1:F:18:HIS:HB2	2.18	0.44
1:E:166:PRO:HG2	1:E:169:GLU:CG	2.48	0.44
1:A:66:ILE:HB	1:A:90:LYS:HZ2	1.82	0.44
1:F:300:ASP:HB3	1:F:303:ARG:HG3	2.00	0.44
1:D:283:ARG:NH2	1:F:156:PHE:HE2	2.15	0.44
1:A:47:GLU:C	1:A:49:ARG:N	2.72	0.44
1:A:209:TYR:CD1	1:A:209:TYR:C	2.91	0.44
1:D:192:THR:HB	1:D:345:LYS:NZ	2.32	0.44
1:D:80:GLU:O	1:D:83:LYS:HB2	2.17	0.44
1:D:83:LYS:O	1:D:87:LEU:HD13	2.18	0.44
1:B:124:ASN:C	1:B:126:ARG:H	2.20	0.44
1:F:264:PRO:HA	1:F:269:PHE:CG	2.53	0.44
1:F:92:VAL:HG12	1:F:93:ILE:H	1.82	0.44
1:A:5:MET:HE2	1:A:28:ILE:HG21	1.99	0.44
1:D:6:GLY:C	1:D:69:VAL:HG23	2.38	0.43
1:E:302:GLY:O	1:E:304:PHE:N	2.51	0.43
1:E:95:GLU:HG2	1:E:96:LYS:H	1.82	0.43
1:F:257:ASP:O	1:F:260:ALA:HB3	2.18	0.43
1:A:121:PRO:HB2	1:A:123:GLN:HE21	1.83	0.43
1:D:327:THR:O	1:D:331:ILE:HG13	2.18	0.43
1:E:147:ILE:HD13	1:E:240:HIS:O	2.17	0.43
1:B:153:ILE:N	1:B:153:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:MET:O	1:E:120:MET:HG3	2.18	0.43
1:F:209:TYR:C	1:F:209:TYR:CD1	2.92	0.43
1:D:209:TYR:CD1	1:D:210:PHE:N	2.86	0.43
1:B:314:ASN:O	1:B:316:ALA:N	2.51	0.43
1:B:183:MET:HG3	1:B:222:ILE:CD1	2.42	0.43
1:D:109:LEU:HD23	1:D:109:LEU:C	2.39	0.43
1:B:229:ILE:HG22	1:B:229:ILE:O	2.18	0.43
1:B:259:LYS:HZ3	1:E:286:ASN:HD21	1.66	0.43
1:E:71:ILE:HB	1:E:93:ILE:O	2.18	0.43
1:A:180:MET:HG2	1:A:184:ILE:HD12	2.00	0.43
1:C:7:PHE:HB2	1:C:33:ILE:HG12	2.00	0.43
1:B:242:THR:HA	1:C:229:ILE:HG21	2.00	0.43
1:C:101:THR:HA	1:C:333:GLU:OE1	2.18	0.43
1:A:86:ILE:O	1:A:88:ALA:O	2.37	0.43
1:D:75:ALA:HA	1:D:78:HIS:ND1	2.34	0.43
1:D:73:THR:HG21	1:D:81:LEU:HD12	2.01	0.43
1:E:196:ASP:HB3	1:E:211:ASP:HB3	1.99	0.43
1:E:121:PRO:HG2	1:E:320:VAL:HG11	2.00	0.43
1:B:164:GLU:HA	1:B:205:ALA:HA	2.00	0.43
1:A:310:ASP:O	1:A:314:ASN:HB2	2.19	0.43
1:A:274:PRO:HA	1:A:277:TYR:CD1	2.54	0.43
1:C:88:ALA:O	1:C:90:LYS:N	2.50	0.43
1:C:235:PRO:HG2	1:C:238:ILE:HG13	2.01	0.43
1:D:221:LYS:HG2	1:D:221:LYS:O	2.19	0.43
1:F:16:ARG:HH11	1:F:259:LYS:HG2	1.84	0.43
1:D:153:ILE:HD13	1:D:236:ARG:CZ	2.48	0.43
1:F:16:ARG:HG2	1:F:17:TYR:CE1	2.54	0.43
1:F:181:ASP:HB2	1:F:328:ASN:HD21	1.84	0.43
1:D:39:ASN:ND2	1:D:42:LEU:HG	2.34	0.43
1:C:68:VAL:HB	1:C:91:SER:HB2	2.01	0.43
1:A:309:TYR:O	1:A:313:VAL:HG12	2.19	0.42
1:E:253:GLN:HE22	1:E:256:ASN:ND2	2.06	0.42
1:A:193:VAL:HG23	1:A:346:LEU:HD21	2.00	0.42
1:E:118:VAL:HG21	1:E:312:ILE:CD1	2.49	0.42
1:E:172:PHE:CE1	1:E:212:VAL:HG21	2.54	0.42
1:C:323:GLU:HG2	1:C:323:GLU:H	1.64	0.42
1:D:85:VAL:HG22	1:D:92:VAL:HG22	2.00	0.42
1:D:99:CYS:SG	1:D:105:ALA:HA	2.60	0.42
1:F:264:PRO:HA	1:F:269:PHE:CD2	2.54	0.42
1:B:260:ALA:O	1:B:262:ILE:HG13	2.19	0.42
1:A:197:ILE:O	1:A:198:ARG:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:GLN:O	1:D:258:LEU:HD22	2.19	0.42
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.88	0.42
1:B:313:VAL:HG22	1:B:313:VAL:O	2.19	0.42
1:D:309:TYR:CE2	1:D:313:VAL:HG11	2.54	0.42
1:F:134:VAL:HG11	1:F:237:PHE:HB3	2.01	0.42
1:D:172:PHE:CE2	1:D:332:LEU:HD12	2.54	0.42
1:D:18:HIS:CE1	1:D:122:TYR:CE2	3.08	0.42
1:F:42:LEU:C	1:F:44:ALA:H	2.23	0.42
1:C:273:SER:HB3	1:D:293:GLN:HB2	2.02	0.42
1:C:190:PRO:O	1:C:346:LEU:HB2	2.19	0.42
1:D:214:LEU:HD12	1:D:222:ILE:CD1	2.49	0.42
1:B:134:VAL:O	1:B:138:VAL:HG23	2.19	0.42
1:F:49:ARG:O	1:F:51:VAL:N	2.43	0.42
1:B:120:MET:HA	1:B:121:PRO:HD3	1.84	0.42
1:D:44:ALA:N	1:D:45:PRO:HD2	2.34	0.42
1:F:148:GLU:C	1:F:149:ILE:HG22	2.40	0.42
1:C:152:HIS:HD2	1:C:154:ASP:OD2	2.02	0.42
1:C:184:ILE:C	1:C:186:LEU:H	2.23	0.42
1:F:344:TYR:CE2	1:F:346:LEU:HD13	2.54	0.42
1:D:161:ILE:H	1:D:161:ILE:HD12	1.85	0.42
1:D:209:TYR:CD1	1:D:209:TYR:C	2.93	0.42
1:A:14:ALA:HB2	1:A:72:CYS:SG	2.59	0.42
1:C:189:ARG:HH22	1:C:330:GLU:CD	2.23	0.42
1:B:47:GLU:C	1:B:49:ARG:N	2.72	0.42
1:B:46:TYR:C	1:B:51:VAL:CG1	2.88	0.42
1:D:316:ALA:HB1	1:D:317:PRO:HD2	2.01	0.42
1:B:220:LEU:HD12	1:B:221:LYS:N	2.34	0.42
1:F:246:PHE:HA	1:F:279:ILE:O	2.19	0.42
1:E:309:TYR:O	1:E:313:VAL:HG12	2.20	0.42
1:E:208:ASN:O	1:E:228:HIS:HD2	2.03	0.42
1:D:131:PHE:CG	1:D:182:ARG:HD2	2.55	0.42
1:F:192:THR:OG1	1:F:193:VAL:N	2.53	0.42
1:F:124:ASN:C	1:F:126:ARG:H	2.23	0.42
1:D:110:ALA:C	1:D:112:GLY:N	2.71	0.42
1:C:283:ARG:HG3	1:C:283:ARG:NH1	2.34	0.42
1:D:253:GLN:NE2	1:D:256:ASN:HD22	2.17	0.42
1:B:109:LEU:HD13	1:B:322:ASP:HB3	2.02	0.42
1:D:83:LYS:O	1:D:86:ILE:HB	2.20	0.42
1:A:228:HIS:C	1:A:229:ILE:HD12	2.40	0.42
1:D:223:LYS:HZ1	1:F:225:LYS:HZ3	1.68	0.42
1:B:209:TYR:C	1:B:209:TYR:CD1	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:HIS:CE1	1:B:77:THR:HG23	2.54	0.42
1:D:25:ARG:HH12	1:D:302:GLY:C	2.23	0.41
1:F:125:ARG:HD2	1:F:178:HIS:CG	2.55	0.41
1:B:265:GLU:HG2	1:B:266:SER:N	2.34	0.41
1:E:118:VAL:HG21	1:E:312:ILE:HD11	2.01	0.41
1:E:25:ARG:HG2	1:E:25:ARG:HH11	1.85	0.41
1:D:6:GLY:O	1:D:69:VAL:HA	2.21	0.41
1:C:92:VAL:HG23	1:C:119:VAL:HG22	2.01	0.41
1:D:333:GLU:O	1:D:335:GLY:N	2.53	0.41
1:A:153:ILE:HG13	1:A:179:THR:HG21	2.02	0.41
1:A:157:ARG:HB3	1:A:160:SER:HB2	2.01	0.41
1:A:130:ASP:N	1:A:130:ASP:OD1	2.52	0.41
1:A:259:LYS:NZ	1:C:286:ASN:HD21	2.18	0.41
1:F:152:HIS:HD2	1:F:154:ASP:OD2	2.03	0.41
1:B:165:ALA:HB1	1:B:166:PRO:CD	2.46	0.41
1:D:32:THR:HG23	1:D:60:LEU:HD13	2.01	0.41
1:E:191:ASN:HD22	1:E:217:GLY:N	2.16	0.41
1:B:58:ASP:C	1:B:60:LEU:H	2.24	0.41
1:A:328:ASN:O	1:A:332:LEU:HB2	2.20	0.41
1:F:167:LYS:H	1:F:167:LYS:HD3	1.84	0.41
1:C:195:TYR:O	1:C:341:PRO:HA	2.21	0.41
1:C:68:VAL:HA	1:C:91:SER:O	2.20	0.41
1:B:57:LEU:O	1:B:61:LEU:HD23	2.21	0.41
1:A:196:ASP:HB3	1:A:211:ASP:HB3	2.02	0.41
1:D:214:LEU:HB2	1:D:222:ILE:CG1	2.50	0.41
1:D:180:MET:O	1:D:184:ILE:HG13	2.20	0.41
1:D:210:PHE:CD1	1:D:210:PHE:C	2.94	0.41
1:E:253:GLN:HE21	1:F:292:LYS:HZ2	1.67	0.41
1:B:153:ILE:O	1:B:226:THR:HG23	2.20	0.41
1:D:19:LEU:HD13	1:D:46:TYR:CZ	2.54	0.41
1:A:29:LYS:CE	1:A:31:LYS:HZ1	2.34	0.41
1:B:293:GLN:OE1	1:F:273:SER:HB3	2.21	0.41
1:D:302:GLY:O	1:D:304:PHE:N	2.54	0.41
1:F:168:GLU:HA	1:F:173:TYR:CD2	2.56	0.41
1:A:68:VAL:HG23	1:A:91:SER:HB2	2.03	0.41
1:B:210:PHE:CE2	1:B:226:THR:HB	2.56	0.41
1:C:69:VAL:HG22	1:C:70:THR:N	2.36	0.41
1:B:23:LYS:HD3	1:B:49:ARG:NH2	2.36	0.41
1:B:157:ARG:O	1:B:160:SER:HB2	2.21	0.41
1:B:147:ILE:HD11	1:C:229:ILE:HB	2.03	0.41
1:C:229:ILE:O	1:C:229:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLU:CD	1:C:103:GLU:H	2.24	0.41
1:F:146:ILE:CD1	1:F:146:ILE:N	2.83	0.41
1:C:253:GLN:CA	1:C:253:GLN:HE21	2.33	0.41
1:F:322:ASP:O	1:F:325:ALA:HB3	2.20	0.41
1:F:333:GLU:C	1:F:335:GLY:H	2.25	0.41
1:E:91:SER:HB3	1:E:118:VAL:HG23	2.03	0.41
1:E:12:LYS:N	1:E:12:LYS:HD3	2.30	0.40
1:D:345:LYS:C	1:D:346:LEU:HD12	2.42	0.40
1:B:286:ASN:HD21	1:F:259:LYS:NZ	2.19	0.40
1:A:149:ILE:HG23	1:A:222:ILE:CG1	2.51	0.40
1:C:3:LEU:HD23	1:C:28:ILE:CD1	2.45	0.40
1:C:96:LYS:NZ	1:C:178:HIS:NE2	2.66	0.40
1:C:221:LYS:HE2	1:C:223:LYS:HG2	2.02	0.40
1:B:296:THR:HA	1:B:297:PRO:HD3	1.88	0.40
1:D:268:GLY:O	1:D:271:GLU:HB2	2.20	0.40
1:B:35:VAL:O	1:B:55:THR:HG22	2.21	0.40
1:F:214:LEU:O	1:F:216:TYR:HD2	2.05	0.40
1:B:189:ARG:NH2	1:B:330:GLU:OE2	2.54	0.40
1:D:214:LEU:O	1:D:216:TYR:CD2	2.75	0.40
1:D:102:VAL:HG12	1:D:333:GLU:OE1	2.22	0.40
1:C:5:MET:HA	1:C:68:VAL:O	2.21	0.40
1:B:59:GLU:HG2	1:B:59:GLU:O	2.21	0.40
1:E:99:CYS:SG	1:E:104:HIS:HB3	2.61	0.40
1:F:11:GLY:CA	1:F:15:ASN:HD22	2.34	0.40
1:A:180:MET:HB2	1:A:224:LEU:HD13	2.02	0.40
1:E:101:THR:HA	1:E:333:GLU:OE1	2.20	0.40
1:C:113:ARG:HH11	1:C:113:ARG:HB2	1.85	0.40
1:F:195:TYR:OH	1:F:331:ILE:HG23	2.22	0.40
1:D:313:VAL:CG1	1:D:314:ASN:N	2.84	0.40
1:D:147:ILE:HD11	1:D:242:THR:CG2	2.46	0.40
1:B:150:GLU:HG2	1:B:152:HIS:CE1	2.57	0.40
1:C:253:GLN:NE2	1:C:256:ASN:HD22	2.16	0.40
1:A:277:TYR:CE2	1:A:295:LYS:HG2	2.57	0.40
1:E:302:GLY:C	1:E:304:PHE:N	2.75	0.40
1:C:310:ASP:O	1:C:316:ALA:HB3	2.22	0.40
1:C:177:ILE:O	1:C:177:ILE:HD13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	348/353 (99%)	325 (93%)	22 (6%)	1 (0%)	46 72
1	B	348/353 (99%)	316 (91%)	26 (8%)	6 (2%)	11 22
1	C	334/353 (95%)	290 (87%)	39 (12%)	5 (2%)	13 26
1	D	340/353 (96%)	292 (86%)	39 (12%)	9 (3%)	7 11
1	E	291/353 (82%)	252 (87%)	31 (11%)	8 (3%)	6 10
1	F	280/353 (79%)	227 (81%)	42 (15%)	11 (4%)	4 5
All	All	1941/2118 (92%)	1702 (88%)	199 (10%)	40 (2%)	9 16

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	GLU
1	C	160	SER
1	D	196	ASP
1	D	200	ASN
1	E	31	LYS
1	E	32	THR
1	F	337	ALA
1	A	203	GLU
1	B	125	ARG
1	C	10	PHE
1	C	153	ILE
1	C	174	SER
1	C	203	GLU
1	D	98	PHE
1	D	153	ILE
1	D	160	SER
1	E	12	LYS
1	E	203	GLU
1	F	34	PHE
1	F	153	ILE

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Mol	Chain	Res	Type
1	B	50	GLY
1	B	160	SER
1	B	315	GLY
1	E	33	ILE
1	F	24	THR
1	F	38	ILE
1	D	303	ARG
1	D	334	ASN
1	E	303	ARG
1	F	125	ARG
1	D	219	GLN
1	E	23	LYS
1	E	74	PRO
1	F	8	ILE
1	F	27	ASN
1	F	334	ASN
1	D	88	ALA
1	B	153	ILE
1	F	141	GLY
1	F	50	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	291/301 (97%)	271 (93%)	20 (7%)	19 38
1	B	294/301 (98%)	271 (92%)	23 (8%)	16 30
1	C	276/301 (92%)	251 (91%)	25 (9%)	12 22
1	D	290/301 (96%)	281 (97%)	9 (3%)	47 76
1	E	232/301 (77%)	211 (91%)	21 (9%)	12 22
1	F	208/301 (69%)	196 (94%)	12 (6%)	25 49
All	All	1591/1806 (88%)	1481 (93%)	110 (7%)	19 38

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	24	THR
1	A	32	THR
1	A	48	GLU
1	A	54	THR
1	A	73	THR
1	A	83	LYS
1	A	87	LEU
1	A	92	VAL
1	A	106	LYS
1	A	134	VAL
1	A	163	HIS
1	A	192	THR
1	A	222	ILE
1	A	225	LYS
1	A	245	SER
1	A	247	ILE
1	A	258	LEU
1	A	332	LEU
1	A	345	LYS
1	B	12	LYS
1	B	26	ASN
1	B	32	THR
1	B	36	ARG
1	B	58	ASP
1	B	64	LYS
1	B	69	VAL
1	B	85	VAL
1	B	87	LEU
1	B	92	VAL
1	B	100	ASP
1	B	113	ARG
1	B	130	ASP
1	B	134	VAL
1	B	139	GLU
1	B	153	ILE
1	B	184	ILE
1	B	222	ILE
1	B	225	LYS
1	B	258	LEU
1	B	265	GLU
1	B	295	LYS
1	B	345	LYS

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Mol	Chain	Res	Type
1	C	2	THR
1	C	12	LYS
1	C	32	THR
1	C	61	LEU
1	C	92	VAL
1	C	96	LYS
1	C	104	HIS
1	C	108	LEU
1	C	111	LEU
1	C	115	LYS
1	C	130	ASP
1	C	134	VAL
1	C	139	GLU
1	C	149	ILE
1	C	177	ILE
1	C	192	THR
1	C	198	ARG
1	C	203	GLU
1	C	207	ASP
1	C	209	TYR
1	C	219	GLN
1	C	221	LYS
1	C	225	LYS
1	C	258	LEU
1	C	281	LYS
1	D	84	LYS
1	D	96	LYS
1	D	177	ILE
1	D	192	THR
1	D	258	LEU
1	D	298	LEU
1	D	310	ASP
1	D	321	LYS
1	D	342	SER
1	E	12	LYS
1	E	27	ASN
1	E	71	ILE
1	E	96	LYS
1	E	130	ASP
1	E	134	VAL
1	E	147	ILE
1	E	149	ILE

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Mol	Chain	Res	Type
1	E	163	HIS
1	E	184	ILE
1	E	192	THR
1	E	203	GLU
1	E	222	ILE
1	E	225	LYS
1	E	271	GLU
1	E	273	SER
1	E	283	ARG
1	E	295	LYS
1	E	298	LEU
1	E	310	ASP
1	E	322	ASP
1	F	130	ASP
1	F	139	GLU
1	F	140	GLN
1	F	149	ILE
1	F	167	LYS
1	F	192	THR
1	F	203	GLU
1	F	222	ILE
1	F	225	LYS
1	F	248	LYS
1	F	258	LEU
1	F	283	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	123	GLN
1	A	152	HIS
1	A	191	ASN
1	A	228	HIS
1	A	253	GLN
1	A	286	ASN
1	A	314	ASN
1	B	26	ASN
1	B	104	HIS
1	B	152	HIS
1	B	191	ASN
1	B	228	HIS

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Mol	Chain	Res	Type
1	B	253	GLN
1	B	286	ASN
1	B	314	ASN
1	C	67	GLN
1	C	152	HIS
1	C	253	GLN
1	C	286	ASN
1	C	314	ASN
1	C	334	ASN
1	D	39	ASN
1	D	62	ASN
1	D	67	GLN
1	D	123	GLN
1	D	140	GLN
1	D	152	HIS
1	D	163	HIS
1	D	191	ASN
1	D	228	HIS
1	D	253	GLN
1	D	256	ASN
1	D	286	ASN
1	E	27	ASN
1	E	152	HIS
1	E	191	ASN
1	E	228	HIS
1	E	253	GLN
1	E	286	ASN
1	E	328	ASN
1	E	334	ASN
1	F	15	ASN
1	F	26	ASN
1	F	136	GLN
1	F	140	GLN
1	F	152	HIS
1	F	191	ASN
1	F	208	ASN
1	F	218	ASN
1	F	243	ASN
1	F	253	GLN
1	F	286	ASN
1	F	328	ASN
1	F	334	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

There are no ligands in this entry.

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, 95^{th} 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	350/353 (99%)	0.09	3 (0%) 85 83	23, 45, 69, 87	0
1	B	350/353 (99%)	0.10	5 (1%) 78 74	36, 56, 75, 94	0
1	C	340/353 (96%)	0.51	28 (8%) 14 10	32, 65, 91, 97	0
1	D	344/353 (97%)	0.39	20 (5%) 26 20	34, 67, 90, 97	0
1	E	297/353 (84%)	0.49	30 (10%) 9 5	26, 58, 97, 99	0
1	F	294/353 (83%)	0.82	44 (14%) 3 2	41, 80, 98, 99	0
All	All	1975/2118 (93%)	0.38	130 (6%) 22 16	23, 60, 95, 99	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	351	LEU	7.0
1	F	35	VAL	6.7
1	F	60	LEU	6.2
1	E	32	THR	5.5
1	C	161	ILE	5.5
1	F	90	LYS	5.4
1	F	34	PHE	5.1
1	A	162	THR	5.0
1	E	119	VAL	4.9
1	F	54	THR	4.7
1	C	3	LEU	4.5
1	D	119	VAL	4.5
1	F	10	PHE	4.4
1	F	118	VAL	4.3
1	F	36	ARG	4.2
1	E	116	GLY	4.1
1	E	117	VAL	4.1
1	B	161	ILE	4.0
1	F	37	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	46	TYR	3.9
1	C	2	THR	3.8
1	E	79	TYR	3.8
1	F	8	ILE	3.7
1	E	33	ILE	3.7
1	C	28	ILE	3.7
1	F	42	LEU	3.7
1	C	312	ILE	3.7
1	F	43	ALA	3.6
1	C	44	ALA	3.6
1	F	92	VAL	3.6
1	F	26	ASN	3.5
1	D	205	ALA	3.5
1	F	270	GLY	3.5
1	C	79	TYR	3.5
1	E	30	VAL	3.5
1	E	118	VAL	3.5
1	C	51	VAL	3.5
1	E	24	THR	3.4
1	F	38	ILE	3.3
1	D	79	TYR	3.3
1	F	9	GLY	3.3
1	D	117	VAL	3.3
1	C	111	LEU	3.2
1	C	92	VAL	3.2
1	F	32	THR	3.2
1	F	82	ALA	3.2
1	F	89	GLY	3.1
1	D	311	THR	3.1
1	E	94	VAL	3.1
1	D	336	PHE	3.1
1	F	158	PRO	3.1
1	F	95	GLU	3.1
1	F	39	ASN	3.1
1	F	329	ILE	3.0
1	E	76	HIS	3.0
1	A	161	ILE	3.0
1	F	160	SER	2.9
1	F	347	GLU	2.9
1	F	22	LEU	2.9
1	D	308	ALA	2.9
1	E	15	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	93	ILE	2.8
1	E	107	GLU	2.8
1	F	46	TYR	2.8
1	E	91	SER	2.8
1	C	30	VAL	2.8
1	C	40	GLU	2.8
1	C	115	LYS	2.8
1	D	116	GLY	2.8
1	E	108	LEU	2.8
1	B	113	ARG	2.8
1	F	41	GLU	2.7
1	D	222	ILE	2.7
1	F	68	VAL	2.7
1	F	19	LEU	2.7
1	D	86	ILE	2.7
1	C	89	GLY	2.7
1	E	92	VAL	2.7
1	E	25	ARG	2.7
1	E	350	HIS	2.7
1	C	205	ALA	2.7
1	D	337	ALA	2.7
1	C	116	GLY	2.7
1	D	75	ALA	2.7
1	E	105	ALA	2.6
1	E	98	PHE	2.6
1	F	16	ARG	2.5
1	B	205	ALA	2.5
1	B	164	GLU	2.5
1	E	100	ASP	2.5
1	E	31	LYS	2.5
1	F	268	GLY	2.5
1	C	108	LEU	2.5
1	C	119	VAL	2.5
1	E	78	HIS	2.5
1	F	214	LEU	2.4
1	D	50	GLY	2.4
1	F	161	ILE	2.4
1	F	302	GLY	2.4
1	D	203	GLU	2.4
1	A	163	HIS	2.4
1	F	91	SER	2.4
1	B	163	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	72	CYS	2.3
1	D	346	LEU	2.3
1	E	19	LEU	2.3
1	F	50	GLY	2.3
1	C	309	TYR	2.3
1	F	21	TYR	2.3
1	E	309	TYR	2.3
1	F	27	ASN	2.2
1	C	117	VAL	2.2
1	F	321	LYS	2.2
1	E	163	HIS	2.2
1	D	318	LYS	2.1
1	D	89	GLY	2.1
1	D	111	LEU	2.1
1	C	38	ILE	2.1
1	C	163	HIS	2.1
1	F	186	LEU	2.1
1	D	312	ILE	2.1
1	C	98	PHE	2.1
1	C	202	VAL	2.1
1	E	13	SER	2.1
1	F	4	THR	2.1
1	C	311	THR	2.0
1	D	102	VAL	2.0
1	C	7	PHE	2.0
1	E	121	PRO	2.0
1	F	23	LYS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.