Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:04 AM GMT

PDB ID	:	2P9N
Title	:	Crystal Structure of bovine Arp2/3 complex co-crystallized with ADP
Authors	:	Nolen, B.J.; Pollard, T.D.
Deposited on	:	2007-03-26
Resolution	:	2.85 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:

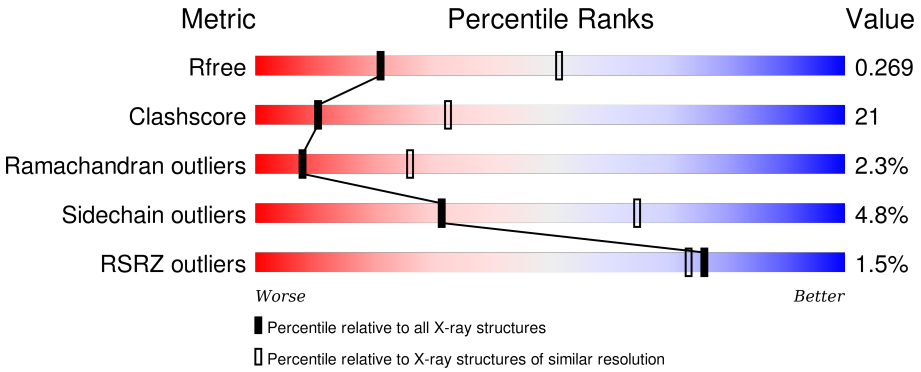
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	418	2% 57% 34% 5%
2	B	394	2% 29% 18% 48%
3	C	372	% 54% 35% 8%
4	D	300	64% 29% 6%
5	E	178	3% 54% 38%

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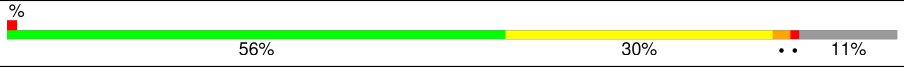
Mol	Chain	Length	Quality of chain
6	F	168	
7	G	151	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13541 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 Actin-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3177	2042	528	592	15			

- Molecule 2 is a protein called Actin-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	203	Total	C	N	O	S	0	0	0
			1572	1006	268	294	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	341	Total	C	N	O	S	0	0	0
			2648	1680	464	485	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	VAL	ILE	CONFLICT	UNP Q58CQ2

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	283	Total	C	N	O	S	0	0	0
			2287	1453	396	430	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	173	Total	C	N	O	S	0	0	0
			1408	904	235	260	9			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	134	Total	C	N	O	S	0	0	0
			1023	642	179	199	3			

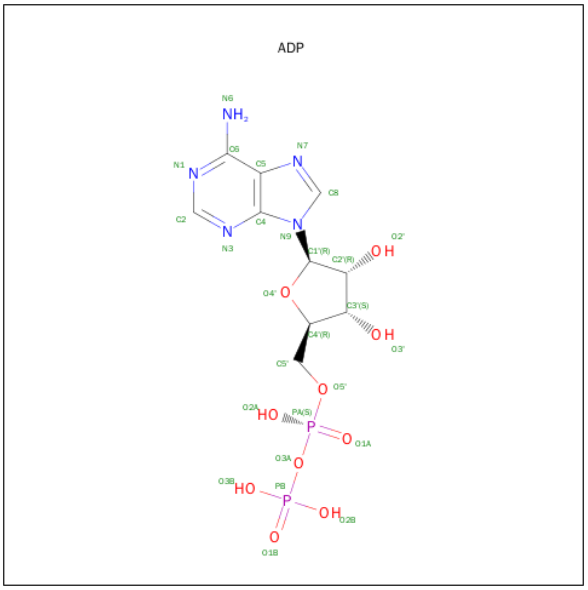
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ASP	GLY	CONFLICT	UNP Q3SYX9
G	28	ASP	GLU	CONFLICT	UNP Q3SYX9

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



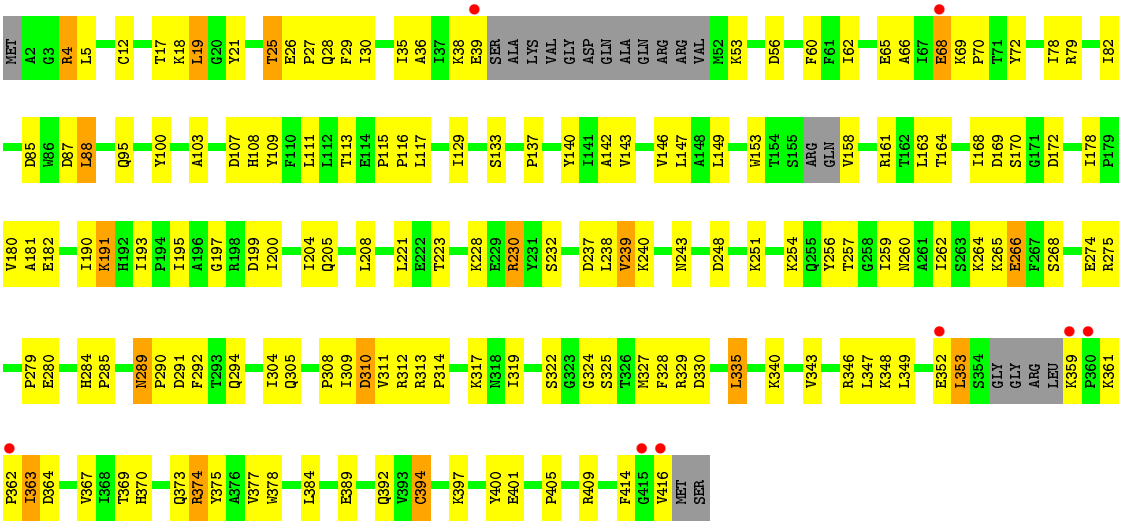
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

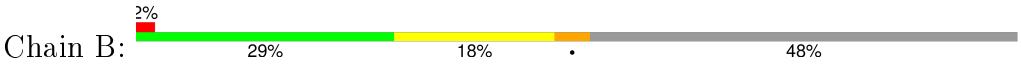
- Molecule 1: Actin-like protein 3

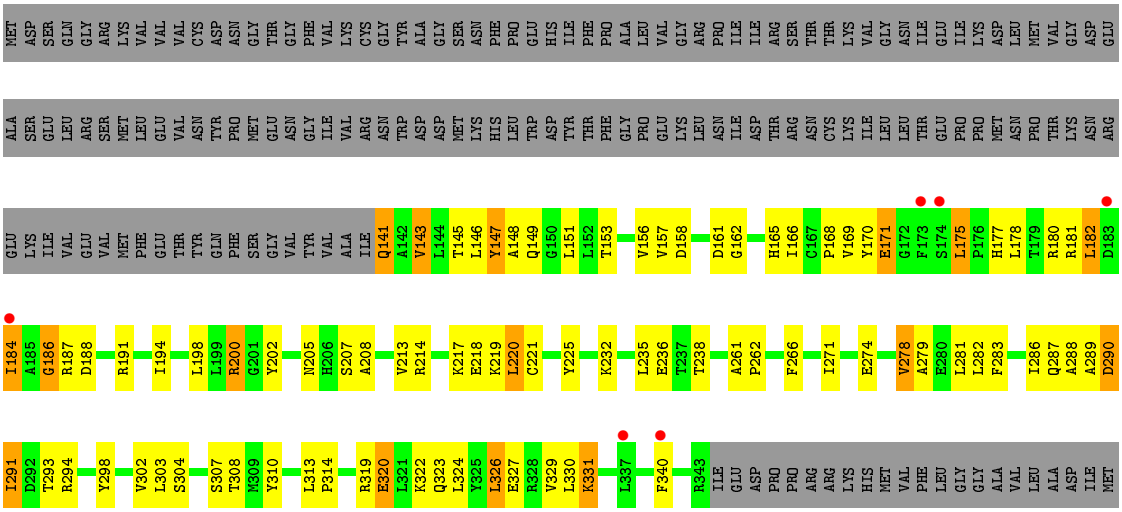
Chain A:



- Molecule 2: Actin-like protein 2

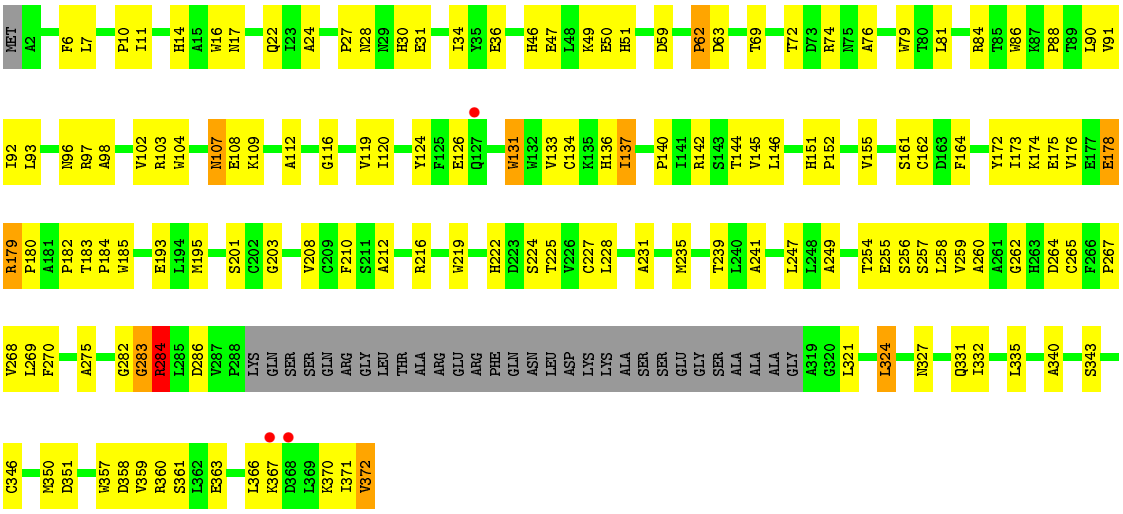
Chain B:





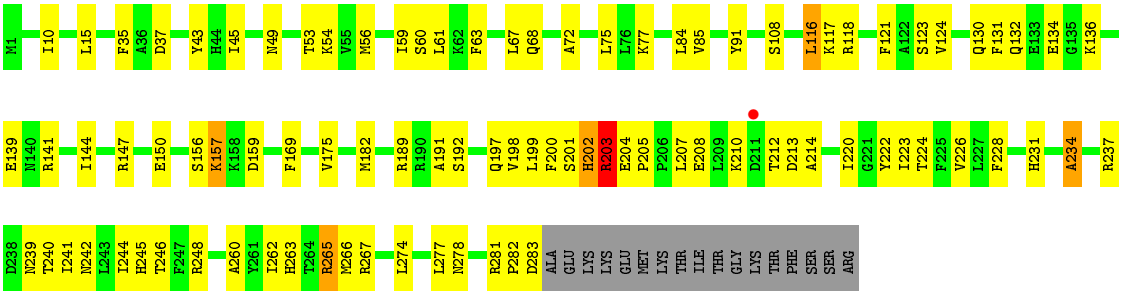
• Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C:



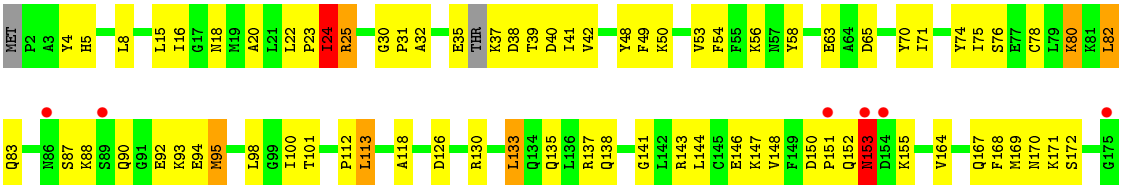
• Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:



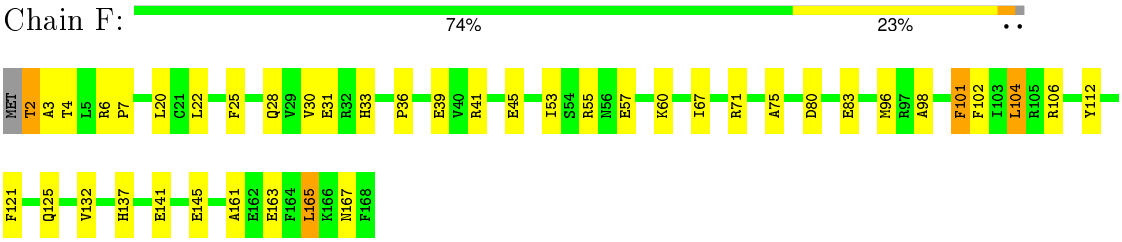
• Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:



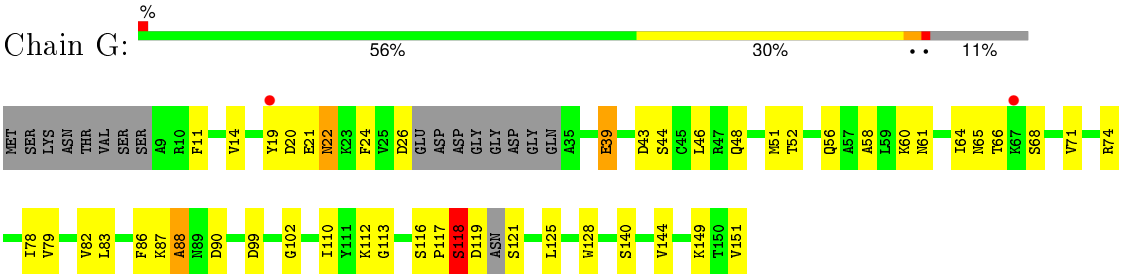
• Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:



- Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.13Å 129.27Å 203.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 46.83 – 2.84	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.85) 92.6 (46.83-2.84)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.272 0.229 , 0.269	Depositor DCC
R_{free} test set	3269 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 68473 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13541	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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

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

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	0.41	0/3257	0.63	0/4418
2	B	0.36	0/1600	0.64	0/2167
3	C	0.40	0/2717	0.68	3/3688 (0.1%)
4	D	0.41	0/2336	0.64	1/3154 (0.0%)
5	E	0.36	0/1441	0.60	0/1941
6	F	0.43	0/1393	0.68	1/1868 (0.1%)
7	G	0.48	1/1034 (0.1%)	0.67	2/1389 (0.1%)
All	All	0.40	1/13778 (0.0%)	0.65	7/18625 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	118	SER	C-O	-5.56	1.12	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	116	SER	C-N-CD	7.62	144.41	128.40
4	D	204	GLU	N-CA-C	-7.43	90.94	111.00
6	F	101	PHE	N-CA-C	-5.40	96.42	111.00
3	C	137	ILE	N-CA-C	-5.32	96.64	111.00
3	C	283	GLY	N-CA-C	5.30	126.36	113.10
3	C	11	ILE	N-CA-C	-5.09	97.26	111.00
7	G	118	SER	CA-C-N	5.01	128.23	117.20

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	3177	0	3123	146	0
2	B	1572	0	1559	91	0
3	C	2648	0	2602	134	0
4	D	2287	0	2252	72	0
5	E	1408	0	1408	74	0
6	F	1371	0	1410	37	0
7	G	1023	0	1041	45	0
8	A	1	0	0	0	0
9	A	27	0	12	2	0
9	B	27	0	12	8	0
All	All	13541	0	13419	575	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 21.

All (575) 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)
3:C:256:SER:HB2	3:C:372:VAL:HG12	1.20	1.17
3:C:183:THR:HG22	3:C:185:TRP:H	1.08	1.09
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.34	1.08
5:E:88:LYS:H	5:E:153:ASN:ND2	1.52	1.07
4:D:197:GLN:HE21	4:D:199:LEU:HD11	1.23	0.99
5:E:88:LYS:N	5:E:153:ASN:HD21	1.59	0.99
3:C:14:HIS:H	3:C:331:GLN:HE22	1.07	0.96
6:F:121:PHE:O	6:F:125:GLN:HG2	1.70	0.91
3:C:269:LEU:H	3:C:283:GLY:HA3	1.38	0.88
3:C:90:LEU:HD23	3:C:91:VAL:N	1.90	0.86
1:A:309:ILE:HA	1:A:312:ARG:HE	1.41	0.85
1:A:343:VAL:HG21	1:A:363:ILE:HG13	1.59	0.84
3:C:183:THR:HG22	3:C:185:TRP:N	1.92	0.84
3:C:92:ILE:HD12	3:C:92:ILE:H	1.41	0.84
3:C:107:ASN:ND2	3:C:109:LYS:H	1.75	0.83
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.61	0.82
1:A:4:ARG:HB2	1:A:4:ARG:HH11	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.63	0.81
7:G:51:MET:HG3	7:G:87:LYS:NZ	1.95	0.80
4:D:197:GLN:NE2	4:D:199:LEU:HD11	1.97	0.80
5:E:25:ARG:HH12	5:E:38:ASP:HA	1.47	0.79
1:A:363:ILE:H	1:A:363:ILE:HD13	1.46	0.79
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.65	0.78
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.65	0.78
2:B:161:ASP:OD2	9:B:395:ADP:H3'	1.84	0.78
4:D:228:PHE:H	4:D:231:HIS:HD2	1.31	0.78
1:A:257:THR:HG22	1:A:268:SER:HB3	1.66	0.77
3:C:107:ASN:HD22	3:C:107:ASN:C	1.87	0.77
3:C:256:SER:CB	3:C:372:VAL:HG12	2.09	0.77
4:D:132:GLN:HE21	4:D:159:ASP:HA	1.50	0.77
3:C:96:ASN:O	3:C:97:ARG:HD3	1.85	0.77
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.67	0.77
3:C:14:HIS:H	3:C:331:GLN:NE2	1.82	0.77
1:A:324:GLY:O	1:A:327:MET:HG2	1.85	0.76
3:C:201:SER:HB3	7:G:149:LYS:NZ	2.00	0.75
5:E:88:LYS:O	5:E:92:GLU:HB2	1.86	0.75
2:B:205:ASN:HD22	2:B:208:ALA:H	1.34	0.75
1:A:384:LEU:HB3	1:A:414:PHE:CZ	2.22	0.74
3:C:371:ILE:O	3:C:372:VAL:HG23	1.87	0.74
1:A:343:VAL:CG2	1:A:363:ILE:HG13	2.17	0.74
5:E:88:LYS:H	5:E:153:ASN:HD21	0.79	0.74
2:B:330:LEU:O	2:B:331:LYS:HB2	1.88	0.74
5:E:150:ASP:C	5:E:152:GLN:H	1.89	0.73
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.18	0.73
1:A:116:PRO:O	1:A:117:LEU:HB2	1.87	0.73
5:E:152:GLN:HB3	5:E:155:LYS:HZ3	1.53	0.73
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.70	0.73
3:C:371:ILE:HG22	3:C:372:VAL:HG22	1.70	0.73
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.19	0.73
2:B:153:THR:OG1	2:B:171:GLU:N	2.21	0.72
3:C:31:GLU:HG2	3:C:49:LYS:HG2	1.69	0.72
3:C:269:LEU:H	3:C:283:GLY:CA	2.03	0.72
1:A:313:ARG:HH12	1:A:363:ILE:HA	1.55	0.72
2:B:184:ILE:HD13	2:B:271:ILE:CD1	2.20	0.72
1:A:289:ASN:HD22	1:A:290:PRO:N	1.88	0.72
5:E:143:ARG:O	5:E:146:GLU:HG2	1.88	0.72
1:A:363:ILE:CD1	1:A:363:ILE:H	2.03	0.71
1:A:223:THR:HG23	1:A:256:TYR:HE2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:H	6:F:28:GLN:NE2	1.89	0.71
6:F:101:PHE:HB3	6:F:104:LEU:HB2	1.72	0.71
3:C:119:VAL:HG21	3:C:136:HIS:HB3	1.72	0.71
1:A:69:LYS:HB3	1:A:72:TYR:HB2	1.71	0.71
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.73	0.71
4:D:281:ARG:C	4:D:283:ASP:H	1.93	0.70
6:F:4:THR:HG23	6:F:55:ARG:HE	1.56	0.70
2:B:303:LEU:HD12	2:B:308:THR:HB	1.74	0.70
5:E:78:CYS:HA	5:E:95:MET:HE1	1.73	0.70
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.26	0.69
1:A:230:ARG:HB3	1:A:230:ARG:HH11	1.57	0.69
1:A:87:ASP:OD2	4:D:267:ARG:HD2	1.93	0.69
1:A:239:VAL:HG11	5:E:48:TYR:HD1	1.57	0.69
3:C:282:GLY:HA3	3:C:370:LYS:NZ	2.07	0.69
1:A:257:THR:HG22	1:A:268:SER:CB	2.23	0.69
5:E:75:ILE:HG23	5:E:144:LEU:HD11	1.75	0.69
5:E:112:PRO:O	5:E:113:LEU:HB2	1.91	0.69
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.09	0.68
2:B:161:ASP:HB2	9:B:395:ADP:H5'1	1.76	0.68
3:C:144:THR:H	6:F:28:GLN:HE22	1.42	0.67
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.29	0.67
2:B:184:ILE:HD13	2:B:271:ILE:HD11	1.75	0.67
1:A:343:VAL:HG13	1:A:363:ILE:HD11	1.77	0.67
2:B:291:ILE:HA	2:B:294:ARG:HD3	1.76	0.67
1:A:230:ARG:CB	1:A:230:ARG:HH11	2.08	0.67
3:C:14:HIS:N	3:C:331:GLN:HE22	1.89	0.67
1:A:4:ARG:CB	1:A:4:ARG:HH11	2.07	0.67
2:B:182:LEU:HG	2:B:281:LEU:HD12	1.76	0.66
1:A:349:LEU:O	1:A:353:LEU:HB2	1.95	0.66
7:G:20:ASP:OD1	7:G:22:ASN:HB2	1.94	0.66
2:B:205:ASN:HD22	2:B:208:ALA:N	1.94	0.66
2:B:205:ASN:ND2	2:B:208:ALA:H	1.94	0.66
3:C:193:GLU:HB3	3:C:195:MET:CE	2.25	0.66
3:C:119:VAL:HG23	3:C:137:ILE:O	1.96	0.66
4:D:263:HIS:HD2	4:D:266:MET:CE	2.08	0.66
7:G:87:LYS:N	7:G:87:LYS:HD3	2.11	0.65
2:B:291:ILE:HD12	2:B:294:ARG:HH11	1.60	0.65
2:B:147:TYR:C	2:B:149:GLN:H	2.00	0.65
1:A:30:ILE:HD13	1:A:375:TYR:CZ	2.31	0.65
1:A:308:PRO:O	1:A:311:VAL:HG12	1.97	0.65
2:B:165:HIS:NE2	2:B:181:ARG:NE	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:O	1:A:79:ARG:HD2	1.97	0.65
1:A:363:ILE:N	1:A:363:ILE:HD13	2.11	0.65
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.79	0.65
1:A:313:ARG:NH1	1:A:363:ILE:HA	2.10	0.65
7:G:51:MET:HG3	7:G:87:LYS:HZ2	1.60	0.65
5:E:153:ASN:O	5:E:155:LYS:HG3	1.96	0.65
1:A:311:VAL:O	1:A:314:PRO:HD2	1.96	0.65
2:B:205:ASN:HB3	2:B:208:ALA:HB3	1.79	0.65
4:D:182:MET:HG3	4:D:200:PHE:CD1	2.31	0.65
5:E:150:ASP:O	5:E:152:GLN:N	2.29	0.65
4:D:234:ALA:HA	4:D:237:ARG:HD3	1.78	0.65
5:E:76:SER:O	5:E:80:LYS:HD3	1.96	0.65
1:A:359:LYS:NZ	1:A:359:LYS:HB3	2.12	0.65
3:C:131:TRP:O	3:C:131:TRP:HE3	1.81	0.64
3:C:267:PRO:HD2	3:C:286:ASP:HB2	1.80	0.64
4:D:228:PHE:H	4:D:231:HIS:CD2	2.15	0.64
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.79	0.64
3:C:151:HIS:CE1	3:C:152:PRO:HG2	2.33	0.64
6:F:20:LEU:HD12	6:F:132:VAL:HG22	1.80	0.64
4:D:68:GLN:HA	4:D:72:ALA:HB3	1.79	0.64
3:C:212:ALA:HB3	3:C:255:GLU:OE2	1.98	0.64
2:B:166:ILE:CD1	2:B:281:LEU:HD22	2.21	0.63
5:E:74:TYR:OH	5:E:98:LEU:HD12	1.98	0.63
4:D:223:ILE:HD12	4:D:223:ILE:N	2.13	0.63
4:D:202:HIS:O	4:D:203:ARG:HB3	1.99	0.62
4:D:282:PRO:O	4:D:283:ASP:HB2	1.99	0.62
2:B:165:HIS:CD2	2:B:181:ARG:HG2	2.34	0.62
3:C:268:VAL:HA	3:C:284:ARG:H	1.65	0.62
3:C:201:SER:HB3	7:G:149:LYS:HZ3	1.62	0.62
1:A:82:ILE:HD12	1:A:115:PRO:HG3	1.80	0.62
4:D:132:GLN:NE2	4:D:159:ASP:HA	2.14	0.61
1:A:348:LYS:HG2	1:A:352:GLU:OE2	2.00	0.61
2:B:326:LEU:C	2:B:326:LEU:HD23	2.21	0.61
2:B:161:ASP:HA	2:B:186:GLY:HA3	1.81	0.61
6:F:96:MET:O	6:F:96:MET:HG2	1.99	0.61
1:A:27:PRO:HG3	1:A:378:TRP:CD2	2.35	0.61
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.83	0.60
5:E:78:CYS:O	5:E:82:LEU:HD22	2.01	0.60
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.37	0.60
4:D:197:GLN:HB3	4:D:226:VAL:HB	1.83	0.60
3:C:107:ASN:HD22	3:C:109:LYS:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:GLU:OE2	3:C:49:LYS:HE3	2.02	0.60
5:E:24:ILE:CG2	5:E:32:ALA:HB1	2.32	0.59
5:E:146:GLU:HG3	5:E:147:LYS:N	2.17	0.59
1:A:374:ARG:CG	1:A:374:ARG:HH11	2.15	0.59
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.37	0.59
6:F:60:LYS:HE3	6:F:112:TYR:CE2	2.36	0.59
1:A:409:ARG:HD3	2:B:200:ARG:O	2.02	0.59
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.31	0.59
1:A:384:LEU:HB3	1:A:414:PHE:HZ	1.68	0.59
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.85	0.58
6:F:98:ALA:O	6:F:101:PHE:O	2.19	0.58
1:A:361:LYS:HD3	1:A:362:PRO:N	2.19	0.58
6:F:125:GLN:HE21	6:F:125:GLN:HA	1.67	0.58
5:E:167:GLN:NE2	5:E:172:SER:HB2	2.18	0.58
3:C:254:THR:OG1	3:C:372:VAL:HG13	2.04	0.58
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.68	0.58
1:A:289:ASN:HD22	1:A:289:ASN:C	2.08	0.58
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.39	0.58
2:B:153:THR:HG23	2:B:170:TYR:HA	1.85	0.57
4:D:278:ASN:O	4:D:281:ARG:HG3	2.03	0.57
1:A:27:PRO:HG3	1:A:378:TRP:CE3	2.40	0.57
4:D:198:VAL:C	4:D:199:LEU:HD12	2.24	0.57
2:B:175:LEU:HB2	2:B:177:HIS:CE1	2.39	0.57
1:A:228:LYS:O	1:A:232:SER:HB2	2.04	0.57
1:A:309:ILE:HB	1:A:312:ARG:HH21	1.69	0.57
3:C:282:GLY:HA3	3:C:370:LYS:HZ1	1.69	0.57
1:A:374:ARG:NH1	1:A:374:ARG:HG3	2.19	0.57
1:A:28:GLN:HG2	4:D:10:ILE:HD13	1.85	0.57
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.20	0.57
5:E:150:ASP:C	5:E:152:GLN:N	2.58	0.57
3:C:264:ASP:O	3:C:265:CYS:HB2	2.04	0.57
2:B:214:ARG:NH1	2:B:218:GLU:OE2	2.37	0.57
5:E:32:ALA:HB2	5:E:135:GLN:OE1	2.05	0.57
3:C:284:ARG:NH1	3:C:286:ASP:O	2.37	0.56
1:A:304:ILE:HG22	1:A:312:ARG:HG2	1.86	0.56
3:C:107:ASN:HD22	3:C:108:GLU:N	2.02	0.56
1:A:205:GLN:NE2	1:A:221:LEU:HG	2.21	0.56
4:D:121:PHE:O	4:D:124:VAL:HG12	2.06	0.56
1:A:204:ILE:HD12	1:A:228:LYS:HB2	1.86	0.56
4:D:53:THR:C	4:D:54:LYS:HD2	2.26	0.56
1:A:305:GLN:HA	1:A:312:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:THR:C	6:F:4:THR:H	2.08	0.56
3:C:84:ARG:O	3:C:84:ARG:HG2	2.06	0.56
3:C:59:ASP:OD2	3:C:104:TRP:N	2.32	0.56
5:E:83:GLN:NE2	5:E:164:VAL:HG11	2.21	0.56
2:B:232:LYS:O	2:B:236:GLU:HG3	2.05	0.56
6:F:36:PRO:HG2	6:F:39:GLU:HB2	1.87	0.55
1:A:30:ILE:HD13	1:A:375:TYR:OH	2.05	0.55
2:B:322:LYS:HG3	2:B:340:PHE:HZ	1.70	0.55
2:B:329:VAL:HG12	2:B:330:LEU:HD23	1.86	0.55
5:E:112:PRO:O	5:E:113:LEU:CB	2.55	0.55
2:B:158:ASP:HA	2:B:304:SER:O	2.06	0.55
6:F:101:PHE:CB	6:F:104:LEU:HB2	2.35	0.55
2:B:320:GLU:HG3	7:G:11:PHE:HE1	1.71	0.55
1:A:289:ASN:HD22	1:A:290:PRO:CD	2.18	0.55
3:C:17:ASN:HD21	3:C:22:GLN:N	2.05	0.55
3:C:144:THR:N	6:F:28:GLN:NE2	2.55	0.54
3:C:107:ASN:C	3:C:107:ASN:ND2	2.57	0.54
5:E:83:GLN:HE22	5:E:164:VAL:HG11	1.72	0.54
7:G:68:SER:HB3	7:G:71:VAL:CG1	2.37	0.54
5:E:95:MET:HG2	5:E:141:GLY:O	2.07	0.54
3:C:74:ARG:O	3:C:93:LEU:HD12	2.07	0.54
1:A:374:ARG:HG2	1:A:375:TYR:CZ	2.43	0.54
3:C:126:GLU:CG	3:C:131:TRP:HZ3	2.21	0.54
1:A:149:LEU:HD11	1:A:180:VAL:HB	1.90	0.54
3:C:92:ILE:CD1	3:C:92:ILE:H	2.17	0.53
4:D:67:LEU:HD23	4:D:144:ILE:HD12	1.88	0.53
2:B:191:ARG:O	2:B:194:ILE:HB	2.08	0.53
5:E:16:ILE:O	5:E:16:ILE:HG23	2.07	0.53
7:G:87:LYS:N	7:G:87:LYS:CD	2.71	0.53
1:A:18:LYS:HD3	1:A:18:LYS:N	2.24	0.53
4:D:45:ILE:HA	4:D:56:MET:O	2.07	0.53
3:C:371:ILE:HD12	3:C:371:ILE:N	2.24	0.53
3:C:175:GLU:OE1	3:C:175:GLU:N	2.42	0.53
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.44	0.53
6:F:53:ILE:N	6:F:53:ILE:HD12	2.23	0.53
1:A:248:ASP:OD1	1:A:251:LYS:HD3	2.09	0.53
1:A:237:ASP:OD2	1:A:240:LYS:HG3	2.09	0.53
7:G:113:GLY:HA3	7:G:125:LEU:HD11	1.90	0.53
7:G:46:LEU:HD23	7:G:51:MET:CE	2.39	0.53
5:E:25:ARG:NH1	5:E:38:ASP:HA	2.18	0.53
4:D:248:ARG:C	4:D:248:ARG:HD3	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:HA	1:A:343:VAL:HG12	1.90	0.52
3:C:216:ARG:NH1	3:C:255:GLU:O	2.43	0.52
6:F:6:ARG:HB3	6:F:7:PRO:HD3	1.91	0.52
3:C:178:GLU:O	3:C:179:ARG:C	2.47	0.52
5:E:18:ASN:O	5:E:63:GLU:HB3	2.09	0.52
4:D:37:ASP:HB2	4:D:43:TYR:HE1	1.73	0.52
1:A:389:GLU:OE2	1:A:414:PHE:HB2	2.09	0.52
3:C:17:ASN:ND2	3:C:22:GLN:H	2.07	0.52
2:B:283:PHE:O	2:B:287:GLN:HG2	2.10	0.52
2:B:278:VAL:HG13	2:B:279:ALA:N	2.25	0.52
7:G:68:SER:CB	7:G:71:VAL:HG12	2.39	0.52
3:C:249:ALA:CB	3:C:332:ILE:HG22	2.37	0.52
4:D:84:LEU:HD23	4:D:85:VAL:N	2.25	0.52
1:A:329:ARG:O	1:A:330:ASP:HB2	2.10	0.52
2:B:175:LEU:N	2:B:175:LEU:HD23	2.25	0.52
4:D:260:ALA:O	4:D:263:HIS:HB2	2.09	0.52
3:C:69:THR:O	3:C:76:ALA:HA	2.10	0.51
2:B:161:ASP:OD1	2:B:187:ARG:HG3	2.11	0.51
5:E:40:ASP:OD2	5:E:143:ARG:NH2	2.38	0.51
6:F:45:GLU:OE2	6:F:45:GLU:N	2.38	0.51
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.92	0.51
1:A:239:VAL:HG23	1:A:240:LYS:H	1.75	0.51
3:C:228:LEU:HD23	3:C:228:LEU:C	2.31	0.51
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.75	0.51
2:B:279:ALA:CB	2:B:320:GLU:HG2	2.41	0.51
1:A:36:ALA:HB2	1:A:66:ALA:HB1	1.93	0.51
4:D:281:ARG:C	4:D:283:ASP:N	2.63	0.51
1:A:208:LEU:HD21	1:A:274:GLU:OE2	2.11	0.51
1:A:62:ILE:HD11	1:A:100:TYR:CE2	2.45	0.51
1:A:289:ASN:ND2	1:A:291:ASP:H	2.09	0.50
1:A:140:TYR:HB2	1:A:394:CYS:SG	2.51	0.50
2:B:157:VAL:HB	2:B:303:LEU:HD13	1.93	0.50
3:C:10:PRO:HB3	3:C:350:MET:HA	1.91	0.50
2:B:184:ILE:HD13	2:B:271:ILE:HD13	1.92	0.50
4:D:281:ARG:O	4:D:283:ASP:N	2.44	0.50
5:E:169:MET:O	5:E:171:LYS:HG2	2.10	0.50
6:F:80:ASP:OD1	6:F:83:GLU:HG3	2.11	0.50
1:A:164:THR:HG23	1:A:181:ALA:HA	1.93	0.50
7:G:78:ILE:O	7:G:82:VAL:HG23	2.11	0.50
7:G:11:PHE:O	7:G:14:VAL:HG12	2.12	0.50
5:E:144:LEU:O	5:E:148:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:GLU:HB3	3:C:195:MET:HE2	1.91	0.50
1:A:374:ARG:CG	1:A:374:ARG:NH1	2.74	0.50
3:C:257:SER:OG	3:C:372:VAL:N	2.44	0.50
3:C:119:VAL:HG22	3:C:120:ILE:N	2.27	0.50
2:B:147:TYR:O	2:B:149:GLN:N	2.41	0.50
2:B:198:LEU:HA	2:B:202:TYR:O	2.12	0.50
3:C:119:VAL:CG2	3:C:136:HIS:HB3	2.40	0.50
1:A:239:VAL:HG22	5:E:4:TYR:CZ	2.46	0.50
2:B:283:PHE:CE2	2:B:324:LEU:HB3	2.47	0.50
3:C:92:ILE:N	3:C:92:ILE:HD12	2.19	0.50
7:G:52:THR:HG22	7:G:52:THR:O	2.12	0.50
1:A:397:LYS:O	1:A:401:GLU:HG3	2.12	0.50
3:C:258:LEU:HB2	3:C:270:PHE:HB2	1.94	0.50
3:C:124:TYR:CD2	3:C:173:ILE:HG21	2.47	0.49
3:C:16:TRP:CE2	3:C:335:LEU:HD21	2.47	0.49
7:G:44:SER:O	7:G:48:GLN:HG3	2.13	0.49
4:D:156:SER:C	4:D:157:LYS:HD2	2.31	0.49
3:C:343:SER:O	3:C:359:VAL:HG23	2.12	0.49
3:C:72:THR:HA	3:C:98:ALA:HB1	1.93	0.49
5:E:35:GLU:HG3	5:E:37:LYS:O	2.12	0.49
3:C:371:ILE:C	3:C:372:VAL:CG2	2.80	0.49
3:C:14:HIS:HA	3:C:24:ALA:O	2.12	0.49
1:A:309:ILE:HG23	1:A:310:ASP:H	1.77	0.49
3:C:282:GLY:HA3	3:C:370:LYS:HZ3	1.75	0.49
3:C:34:ILE:HB	3:C:46:HIS:HB2	1.95	0.49
4:D:208:GLU:OE2	4:D:208:GLU:N	2.38	0.49
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.95	0.49
1:A:262:ILE:C	1:A:264:LYS:H	2.16	0.49
5:E:152:GLN:HB3	5:E:155:LYS:CE	2.43	0.49
2:B:161:ASP:OD2	9:B:395:ADP:C3'	2.57	0.49
5:E:82:LEU:HB3	5:E:148:VAL:HG11	1.94	0.49
3:C:208:VAL:HG12	3:C:219:TRP:CB	2.43	0.49
5:E:8:LEU:HD12	5:E:41:ILE:HD13	1.94	0.49
5:E:95:MET:HG3	5:E:141:GLY:HA3	1.95	0.48
1:A:12:CYS:HB3	1:A:78:ILE:CD1	2.43	0.48
1:A:359:LYS:HZ3	1:A:359:LYS:HB3	1.78	0.48
6:F:20:LEU:HD12	6:F:132:VAL:CG2	2.42	0.48
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.48	0.48
1:A:343:VAL:O	1:A:347:LEU:HD13	2.13	0.48
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.48	0.48
2:B:310:TYR:CE1	9:B:395:ADP:H2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:240:THR:O	4:D:244:ILE:HG22	2.13	0.48
1:A:108:HIS:O	1:A:137:PRO:HD2	2.13	0.48
3:C:358:ASP:HB3	3:C:361:SER:CB	2.44	0.48
1:A:190:ILE:HG22	1:A:191:LYS:N	2.29	0.48
3:C:183:THR:HG23	3:C:184:PRO:CD	2.41	0.48
4:D:199:LEU:HB2	4:D:224:THR:HB	1.95	0.48
1:A:308:PRO:HG2	2:B:207:SER:HB2	1.95	0.48
5:E:146:GLU:CG	5:E:147:LYS:N	2.77	0.48
5:E:58:TYR:CD1	5:E:168:PHE:HZ	2.32	0.48
1:A:79:ARG:NE	1:A:79:ARG:HA	2.27	0.48
7:G:74:ARG:O	7:G:78:ILE:HG13	2.13	0.48
5:E:90:GLN:O	5:E:93:LYS:HB2	2.13	0.48
3:C:146:LEU:HD11	3:C:162:CYS:SG	2.54	0.47
2:B:161:ASP:OD1	2:B:161:ASP:O	2.32	0.47
3:C:142:ARG:HG3	3:C:142:ARG:HH11	1.78	0.47
5:E:24:ILE:HG23	5:E:32:ALA:HB1	1.97	0.47
4:D:134:GLU:HB2	4:D:136:LYS:HG3	1.96	0.47
1:A:370:HIS:O	1:A:373:GLN:HG3	2.14	0.47
7:G:71:VAL:O	7:G:74:ARG:HB3	2.14	0.47
4:D:203:ARG:HD3	4:D:203:ARG:C	2.34	0.47
1:A:205:GLN:HE22	1:A:221:LEU:HG	1.80	0.47
1:A:319:ILE:HB	1:A:367:VAL:HG22	1.96	0.47
7:G:140:SER:O	7:G:144:VAL:HG23	2.15	0.47
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.41	0.47
6:F:57:GLU:HA	7:G:117:PRO:HG3	1.96	0.47
6:F:2:THR:OG1	6:F:3:ALA:N	2.45	0.47
4:D:202:HIS:O	4:D:203:ARG:CB	2.61	0.47
3:C:324:LEU:HD22	3:C:357:TRP:CH2	2.50	0.47
3:C:133:VAL:O	3:C:134:CYS:HB3	2.15	0.47
3:C:10:PRO:HD2	3:C:28:ASN:ND2	2.30	0.46
1:A:53:LYS:O	1:A:56:ASP:OD2	2.33	0.46
6:F:125:GLN:NE2	6:F:125:GLN:HA	2.31	0.46
7:G:87:LYS:O	7:G:88:ALA:C	2.54	0.46
5:E:38:ASP:N	5:E:38:ASP:OD2	2.44	0.46
2:B:153:THR:HA	2:B:169:VAL:O	2.15	0.46
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.49	0.46
2:B:286:ILE:O	2:B:289:ALA:HB3	2.15	0.46
6:F:161:ALA:O	6:F:165:LEU:HD22	2.15	0.46
3:C:254:THR:HG1	3:C:257:SER:H	1.61	0.46
2:B:279:ALA:HB1	2:B:320:GLU:HG2	1.96	0.46
7:G:64:ILE:HG22	7:G:65:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:HG	1:A:29:PHE:HB2	1.96	0.46
1:A:129:ILE:O	1:A:133:SER:HB2	2.15	0.46
3:C:371:ILE:O	3:C:372:VAL:CG2	2.62	0.46
2:B:266:PHE:HD1	2:B:320:GLU:OE2	1.99	0.46
2:B:303:LEU:HD12	2:B:308:THR:CB	2.43	0.46
4:D:244:ILE:HG23	4:D:245:HIS:N	2.30	0.46
1:A:309:ILE:HG23	1:A:310:ASP:N	2.30	0.46
3:C:126:GLU:CB	3:C:131:TRP:HZ3	2.28	0.46
3:C:79:TRP:CZ3	3:C:88:PRO:HB3	2.50	0.46
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.46	0.46
3:C:208:VAL:HG12	3:C:219:TRP:HB3	1.96	0.46
2:B:182:LEU:HG	2:B:281:LEU:CD1	2.46	0.46
3:C:17:ASN:HD21	3:C:22:GLN:H	1.63	0.46
1:A:170:SER:OG	1:A:325:SER:HB2	2.16	0.46
5:E:126:ASP:OD2	5:E:130:ARG:NH1	2.48	0.46
5:E:100:ILE:HD11	5:E:138:GLN:OE1	2.15	0.46
1:A:289:ASN:ND2	1:A:289:ASN:C	2.69	0.46
7:G:58:ALA:HB1	7:G:79:VAL:HG22	1.98	0.46
4:D:118:ARG:C	4:D:118:ARG:HD3	2.37	0.45
3:C:283:GLY:O	3:C:284:ARG:HB2	2.15	0.45
7:G:66:THR:HG21	7:G:71:VAL:HG21	1.99	0.45
3:C:151:HIS:CG	3:C:152:PRO:HD2	2.51	0.45
4:D:201:SER:O	4:D:202:HIS:C	2.55	0.45
1:A:200:ILE:O	1:A:204:ILE:HG13	2.17	0.45
3:C:173:ILE:O	3:C:176:VAL:HG22	2.17	0.45
1:A:35:ILE:HG21	1:A:88:LEU:HG	1.97	0.45
3:C:6:PHE:O	3:C:7:LEU:HB3	2.15	0.45
2:B:143:VAL:O	2:B:147:TYR:CB	2.64	0.45
1:A:254:LYS:HG2	1:A:275:ARG:NH1	2.31	0.45
3:C:247:LEU:HA	3:C:262:GLY:HA3	1.99	0.45
3:C:225:THR:HG22	3:C:241:ALA:HA	1.99	0.45
7:G:64:ILE:O	7:G:149:LYS:HB3	2.17	0.45
5:E:24:ILE:HG12	5:E:24:ILE:O	2.15	0.45
1:A:274:GLU:OE1	1:A:274:GLU:N	2.44	0.45
7:G:52:THR:O	7:G:56:GLN:HG3	2.17	0.45
2:B:182:LEU:HD11	2:B:278:VAL:N	2.31	0.45
3:C:260:ALA:O	3:C:267:PRO:HA	2.16	0.45
7:G:119:ASP:C	7:G:121:SER:N	2.70	0.45
3:C:145:VAL:HA	3:C:161:SER:HB3	1.99	0.45
2:B:225:TYR:CZ	2:B:319:ARG:HD2	2.51	0.45
3:C:81:LEU:HD13	3:C:86:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:SER:O	7:G:125:LEU:HB2	2.17	0.45
6:F:30:VAL:HB	6:F:33:HIS:HB2	1.99	0.45
7:G:39:GLU:HG2	7:G:78:ILE:CD1	2.47	0.45
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.16	0.45
1:A:285:PRO:HG2	1:A:294:GLN:O	2.16	0.45
1:A:21:TYR:OH	1:A:103:ALA:HB2	2.17	0.45
2:B:146:LEU:O	2:B:151:LEU:O	2.34	0.45
4:D:245:HIS:CE1	4:D:246:THR:HG23	2.52	0.45
4:D:212:THR:C	4:D:214:ALA:H	2.20	0.45
2:B:238:THR:HG22	6:F:106:ARG:NH2	2.32	0.45
7:G:118:SER:O	7:G:119:ASP:CG	2.56	0.44
2:B:283:PHE:CD2	2:B:324:LEU:HB3	2.52	0.44
1:A:193:ILE:HG23	1:A:292:PHE:CE2	2.51	0.44
2:B:180:ARG:HD3	2:B:281:LEU:HD21	1.99	0.44
3:C:116:GLY:HA2	3:C:144:THR:OG1	2.17	0.44
1:A:168:ILE:HD13	1:A:335:LEU:HD11	1.98	0.44
1:A:317:LYS:HE2	1:A:364:ASP:HB3	1.99	0.44
7:G:60:LYS:HE2	7:G:61:ASN:ND2	2.32	0.44
1:A:361:LYS:HD3	1:A:362:PRO:O	2.17	0.44
7:G:110:ILE:CD1	7:G:128:TRP:HB3	2.47	0.44
6:F:163:GLU:O	6:F:167:ASN:ND2	2.50	0.44
5:E:53:VAL:HG13	5:E:54:PHE:N	2.33	0.44
4:D:203:ARG:C	4:D:203:ARG:CD	2.86	0.44
4:D:189:ARG:C	4:D:191:ALA:H	2.19	0.44
5:E:20:ALA:O	5:E:22:LEU:HD22	2.18	0.44
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.53	0.44
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.99	0.44
3:C:183:THR:HG21	3:C:185:TRP:HD1	1.83	0.43
5:E:56:LYS:NZ	5:E:170:ASN:OD1	2.50	0.43
4:D:189:ARG:HA	4:D:192:SER:O	2.18	0.43
1:A:25:THR:HG22	1:A:26:GLU:HG2	2.00	0.43
1:A:309:ILE:HA	1:A:312:ARG:NE	2.20	0.43
1:A:232:SER:HA	1:A:275:ARG:O	2.18	0.43
4:D:131:PHE:CD1	4:D:139:GLU:HG3	2.53	0.43
1:A:343:VAL:HG23	1:A:346:ARG:HH21	1.84	0.43
3:C:74:ARG:HG2	3:C:97:ARG:O	2.18	0.43
1:A:117:LEU:HD13	1:A:190:ILE:HD12	2.00	0.43
2:B:177:HIS:CD2	2:B:177:HIS:H	2.36	0.43
7:G:39:GLU:HG2	7:G:78:ILE:HD13	2.01	0.43
2:B:322:LYS:HG3	2:B:340:PHE:CZ	2.52	0.43
4:D:207:LEU:HA	4:D:210:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:327:ASN:HB2	3:C:351:ASP:HB3	1.99	0.43
1:A:172:ASP:HB2	9:A:501:ADP:O5'	2.18	0.43
1:A:143:VAL:HG13	1:A:146:VAL:CG2	2.48	0.43
6:F:25:PHE:CD1	6:F:67:ILE:HD13	2.53	0.43
3:C:259:VAL:HG12	3:C:332:ILE:CD1	2.49	0.43
7:G:110:ILE:HD11	7:G:128:TRP:HB3	1.99	0.43
4:D:265:ARG:NH1	6:F:145:GLU:OE2	2.51	0.43
4:D:75:LEU:HD13	4:D:123:SER:N	2.34	0.43
3:C:62:PRO:HG2	3:C:63:ASP:H	1.83	0.43
3:C:332:ILE:HA	3:C:346:CYS:O	2.19	0.43
3:C:17:ASN:ND2	3:C:22:GLN:HG3	2.33	0.43
1:A:347:LEU:HD22	1:A:363:ILE:HD12	2.01	0.43
2:B:178:LEU:HD21	2:B:288:ALA:O	2.17	0.43
2:B:153:THR:HG22	2:B:153:THR:O	2.17	0.43
2:B:147:TYR:C	2:B:149:GLN:N	2.68	0.43
6:F:137:HIS:CE1	6:F:141:GLU:HG3	2.53	0.43
1:A:310:ASP:N	1:A:310:ASP:OD1	2.49	0.43
5:E:15:LEU:HD22	5:E:63:GLU:HG3	1.97	0.43
4:D:234:ALA:HB2	4:D:237:ARG:NH1	2.34	0.43
2:B:141:GLN:HE21	2:B:141:GLN:HB3	1.65	0.43
3:C:360:ARG:HA	3:C:363:GLU:OE1	2.18	0.43
3:C:269:LEU:HB3	3:C:283:GLY:HA2	2.01	0.43
6:F:60:LYS:H	6:F:75:ALA:HB3	1.84	0.43
5:E:8:LEU:HD12	5:E:41:ILE:CD1	2.48	0.43
5:E:18:ASN:CG	5:E:118:ALA:H	2.21	0.43
5:E:133:LEU:HB3	5:E:137:ARG:HH12	1.84	0.43
1:A:60:PHE:CE1	1:A:95:GLN:NE2	2.87	0.43
3:C:102:VAL:O	3:C:103:ARG:NH1	2.50	0.43
3:C:102:VAL:O	3:C:103:ARG:HG2	2.18	0.43
1:A:147:LEU:HD12	1:A:377:VAL:HG13	2.01	0.43
1:A:107:ASP:CG	4:D:147:ARG:HH22	2.22	0.42
7:G:68:SER:O	7:G:71:VAL:CG1	2.66	0.42
1:A:143:VAL:HG13	1:A:146:VAL:HG23	2.00	0.42
4:D:15:LEU:HA	4:D:15:LEU:HD23	1.81	0.42
1:A:259:ILE:CD1	1:A:266:GLU:HG3	2.48	0.42
2:B:218:GLU:HG2	9:B:395:ADP:C4	2.54	0.42
1:A:374:ARG:O	1:A:375:TYR:CD2	2.73	0.42
2:B:194:ILE:HG12	2:B:213:VAL:HG21	2.01	0.42
2:B:225:TYR:CE2	2:B:319:ARG:HD2	2.54	0.42
3:C:227:CYS:SG	3:C:239:THR:HG23	2.60	0.42
7:G:99:ASP:O	7:G:102:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:90:LEU:HD23	3:C:91:VAL:H	1.76	0.42
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.42	0.42
1:A:230:ARG:NH1	1:A:230:ARG:HB3	2.31	0.42
6:F:45:GLU:HB3	7:G:24:PHE:CE2	2.54	0.42
5:E:30:GLY:C	5:E:32:ALA:H	2.22	0.42
1:A:17:THR:HG22	1:A:19:LEU:HD23	2.01	0.42
3:C:30:HIS:HB3	3:C:51:HIS:O	2.20	0.42
3:C:254:THR:HA	3:C:340:ALA:O	2.19	0.42
7:G:86:PHE:C	7:G:87:LYS:HD3	2.39	0.42
3:C:201:SER:HB3	7:G:149:LYS:HZ2	1.82	0.42
1:A:109:TYR:CD1	1:A:137:PRO:HG2	2.53	0.42
1:A:369:THR:HA	1:A:373:GLN:OE1	2.20	0.42
4:D:130:GLN:OE1	4:D:130:GLN:HA	2.19	0.42
3:C:107:ASN:ND2	3:C:109:LYS:N	2.57	0.42
2:B:219:LYS:HG2	2:B:220:LEU:CD1	2.48	0.42
1:A:200:ILE:CG2	1:A:228:LYS:HD2	2.50	0.42
1:A:260:ASN:O	1:A:264:LYS:HA	2.19	0.42
5:E:153:ASN:HA	5:E:153:ASN:HD22	1.64	0.42
3:C:332:ILE:O	3:C:332:ILE:HG23	2.19	0.42
1:A:254:LYS:HG2	1:A:275:ARG:HH11	1.83	0.42
3:C:22:GLN:HE21	3:C:36:GLU:HB2	1.84	0.42
2:B:170:TYR:O	2:B:171:GLU:C	2.58	0.42
4:D:223:ILE:N	4:D:223:ILE:CD1	2.81	0.42
2:B:165:HIS:CD2	2:B:181:ARG:HE	2.37	0.42
1:A:328:PHE:CZ	9:A:501:ADP:H2	2.37	0.42
5:E:144:LEU:HD23	5:E:144:LEU:HA	1.94	0.42
5:E:113:LEU:HD11	5:E:169:MET:CE	2.50	0.42
1:A:279:PRO:HG3	1:A:328:PHE:CE1	2.54	0.42
1:A:238:LEU:HD21	1:A:280:GLU:HG2	2.02	0.42
3:C:366:LEU:N	3:C:366:LEU:HD12	2.35	0.42
1:A:153:TRP:CE3	1:A:161:ARG:HD3	2.53	0.42
1:A:308:PRO:CG	2:B:207:SER:HB2	2.49	0.42
2:B:217:LYS:HD2	2:B:310:TYR:OH	2.20	0.42
2:B:217:LYS:O	2:B:221:CYS:HB2	2.19	0.42
1:A:361:LYS:C	1:A:361:LYS:HD3	2.40	0.42
1:A:284:HIS:N	1:A:285:PRO:HD3	2.35	0.42
5:E:5:HIS:HD2	5:E:65:ASP:OD2	2.03	0.42
4:D:213:ASP:OD1	4:D:213:ASP:N	2.51	0.42
1:A:111:LEU:HD23	1:A:111:LEU:C	2.39	0.42
3:C:222:HIS:C	3:C:224:SER:H	2.23	0.42
3:C:47:GLU:HG2	3:C:49:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:PRO:HB2	5:E:171:LYS:HD2	2.02	0.41
4:D:263:HIS:HD2	4:D:266:MET:HE3	1.82	0.41
4:D:239:ASN:HA	4:D:242:ASN:HD22	1.85	0.41
1:A:113:THR:HA	1:A:142:ALA:O	2.20	0.41
4:D:54:LYS:HD2	4:D:54:LYS:N	2.34	0.41
1:A:85:ASP:OD2	1:A:88:LEU:HD22	2.20	0.41
3:C:102:VAL:HA	3:C:112:ALA:O	2.19	0.41
3:C:144:THR:OG1	6:F:28:GLN:NE2	2.44	0.41
5:E:98:LEU:HA	5:E:101:THR:HG23	2.02	0.41
2:B:286:ILE:HD12	2:B:298:TYR:CE2	2.56	0.41
5:E:18:ASN:ND2	5:E:118:ALA:H	2.18	0.41
1:A:335:LEU:HD23	1:A:335:LEU:O	2.19	0.41
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.88	0.41
4:D:60:SER:HB2	4:D:91:TYR:HA	2.02	0.41
1:A:163:LEU:HG	1:A:416:VAL:HG13	2.03	0.41
3:C:183:THR:CG2	3:C:184:PRO:N	2.83	0.41
1:A:116:PRO:HG2	1:A:178:ILE:HD13	2.01	0.41
1:A:62:ILE:HD11	1:A:100:TYR:HE2	1.83	0.41
5:E:8:LEU:HD11	5:E:41:ILE:HA	2.02	0.41
2:B:290:ASP:O	2:B:293:THR:N	2.53	0.41
4:D:274:LEU:HA	4:D:274:LEU:HD23	1.89	0.41
1:A:68:GLU:CD	1:A:68:GLU:H	2.16	0.41
1:A:169:ASP:HA	1:A:322:SER:O	2.21	0.41
2:B:323:GLN:HG2	7:G:14:VAL:HG13	2.03	0.41
1:A:36:ALA:HB1	1:A:72:TYR:HB3	2.01	0.41
5:E:94:GLU:O	5:E:98:LEU:HB2	2.19	0.41
6:F:39:GLU:OE2	6:F:71:ARG:HD3	2.20	0.41
3:C:172:TYR:C	3:C:172:TYR:CD2	2.94	0.41
5:E:42:VAL:HA	5:E:71:ILE:HD13	2.03	0.41
3:C:185:TRP:HE3	3:C:235:MET:CE	2.33	0.41
2:B:330:LEU:HB2	2:B:331:LYS:H	1.54	0.41
5:E:70:TYR:CZ	5:E:133:LEU:HG	2.56	0.41
6:F:125:GLN:CA	6:F:125:GLN:HE21	2.30	0.41
4:D:77:LYS:HA	4:D:77:LYS:HD2	1.80	0.41
2:B:166:ILE:O	2:B:168:PRO:HD3	2.20	0.41
1:A:313:ARG:HB2	1:A:314:PRO:HD3	2.03	0.41
9:B:395:ADP:O1A	9:B:395:ADP:O1B	2.38	0.41
2:B:161:ASP:HB2	9:B:395:ADP:H3'	2.02	0.41
6:F:4:THR:CG2	6:F:55:ARG:HE	2.31	0.41
2:B:326:LEU:HD23	2:B:327:GLU:N	2.36	0.41
1:A:5:LEU:HB3	1:A:108:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:358:ASP:HB3	3:C:361:SER:HB3	2.01	0.41
1:A:400:TYR:CE1	1:A:405:PRO:HB3	2.55	0.41
4:D:35:PHE:CD2	4:D:35:PHE:N	2.88	0.41
1:A:311:VAL:C	1:A:314:PRO:HD2	2.40	0.41
1:A:389:GLU:O	1:A:392:GLN:HB2	2.21	0.41
4:D:169:PHE:HB2	4:D:175:VAL:HG22	2.03	0.41
2:B:161:ASP:HB2	9:B:395:ADP:C5'	2.49	0.40
3:C:358:ASP:HB3	3:C:361:SER:HB2	2.02	0.40
4:D:61:LEU:HD23	4:D:63:PHE:CZ	2.55	0.40
4:D:202:HIS:C	4:D:202:HIS:ND1	2.74	0.40
3:C:174:LYS:CG	3:C:175:GLU:OE1	2.69	0.40
7:G:60:LYS:HE2	7:G:61:ASN:HD22	1.86	0.40
2:B:166:ILE:HD13	2:B:282:LEU:HA	2.03	0.40
3:C:62:PRO:HG2	3:C:108:GLU:OE2	2.22	0.40
7:G:66:THR:HB	7:G:71:VAL:HG11	2.01	0.40
4:D:59:ILE:HB	4:D:116:LEU:HD13	2.02	0.40
3:C:144:THR:CB	6:F:28:GLN:HE21	2.33	0.40
4:D:75:LEU:HD23	4:D:75:LEU:C	2.41	0.40
1:A:195:ILE:HA	1:A:199:ASP:OD2	2.21	0.40
4:D:220:ILE:N	4:D:220:ILE:HD12	2.36	0.40
4:D:262:ILE:HG22	4:D:266:MET:HE2	2.02	0.40
2:B:147:TYR:O	2:B:151:LEU:O	2.39	0.40
4:D:237:ARG:O	4:D:241:ILE:HG13	2.22	0.40
3:C:7:LEU:CD1	3:C:27:PRO:HB2	2.52	0.40
1:A:158:VAL:O	1:A:158:VAL:HG23	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	389/418 (93%)	347 (89%)	36 (9%)	6 (2%)	13 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	201/394 (51%)	164 (82%)	24 (12%)	13 (6%)	1 4
3	C	337/372 (91%)	297 (88%)	34 (10%)	6 (2%)	11 33
4	D	281/300 (94%)	255 (91%)	24 (8%)	2 (1%)	26 59
5	E	169/178 (95%)	136 (80%)	25 (15%)	8 (5%)	3 9
6	F	165/168 (98%)	156 (94%)	8 (5%)	1 (1%)	30 63
7	G	128/151 (85%)	115 (90%)	10 (8%)	3 (2%)	8 26
All	All	1670/1981 (84%)	1470 (88%)	161 (10%)	39 (2%)	8 26

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLU
2	B	147	TYR
2	B	171	GLU
5	E	153	ASN
2	B	145	THR
2	B	186	GLY
2	B	290	ASP
2	B	331	LYS
3	C	203	GLY
7	G	22	ASN
7	G	88	ALA
1	A	265	LYS
2	B	143	VAL
2	B	148	ALA
3	C	284	ARG
4	D	203	ARG
4	D	234	ALA
5	E	49	PHE
5	E	113	LEU
5	E	151	PRO
1	A	70	PRO
1	A	310	ASP
2	B	278	VAL
3	C	50	GLU
3	C	275	ALA
5	E	87	SER
7	G	118	SER
1	A	65	GLU
2	B	307	SER

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Mol	Chain	Res	Type
3	C	179	ARG
6	F	41	ARG
1	A	197	GLY
2	B	184	ILE
5	E	50	LYS
2	B	291	ILE
2	B	162	GLY
3	C	62	PRO
5	E	31	PRO
5	E	24	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/363 (96%)	330 (95%)	17 (5%)	31	63
2	B	164/345 (48%)	155 (94%)	9 (6%)	27	58
3	C	290/313 (93%)	278 (96%)	12 (4%)	37	71
4	D	249/264 (94%)	239 (96%)	10 (4%)	38	72
5	E	155/159 (98%)	147 (95%)	8 (5%)	29	60
6	F	154/155 (99%)	148 (96%)	6 (4%)	39	73
7	G	110/124 (89%)	102 (93%)	8 (7%)	17	42
All	All	1469/1723 (85%)	1399 (95%)	70 (5%)	31	65

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	19	LEU
1	A	25	THR
1	A	39	GLU
1	A	68	GLU
1	A	88	LEU
1	A	182	GLU

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Mol	Chain	Res	Type
1	A	191	LYS
1	A	230	ARG
1	A	239	VAL
1	A	243	ASN
1	A	289	ASN
1	A	335	LEU
1	A	353	LEU
1	A	363	ILE
1	A	374	ARG
1	A	394	CYS
2	B	141	GLN
2	B	175	LEU
2	B	182	LEU
2	B	200	ARG
2	B	220	LEU
2	B	235	LEU
2	B	274	GLU
2	B	320	GLU
2	B	326	LEU
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	164	PHE
3	C	178	GLU
3	C	182	PRO
3	C	210	PHE
3	C	284	ARG
3	C	321	LEU
3	C	324	LEU
3	C	367	LYS
3	C	372	VAL
4	D	49	ASN
4	D	108	SER
4	D	116	LEU
4	D	117	LYS
4	D	141	ARG
4	D	157	LYS
4	D	202	HIS
4	D	203	ARG
4	D	265	ARG
4	D	277	LEU
5	E	24	ILE

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Mol	Chain	Res	Type
5	E	25	ARG
5	E	39	THR
5	E	80	LYS
5	E	82	LEU
5	E	95	MET
5	E	133	LEU
5	E	153	ASN
6	F	2	THR
6	F	22	LEU
6	F	31	GLU
6	F	102	PHE
6	F	104	LEU
6	F	165	LEU
7	G	19	TYR
7	G	21	GLU
7	G	26	ASP
7	G	39	GLU
7	G	43	ASP
7	G	90	ASP
7	G	112	LYS
7	G	151	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	122	ASN
1	A	192	HIS
1	A	243	ASN
1	A	289	ASN
1	A	318	ASN
1	A	370	HIS
1	A	395	HIS
1	A	410	HIS
2	B	141	GLN
2	B	177	HIS
2	B	205	ASN
2	B	284	ASN
2	B	323	GLN
3	C	22	GLN
3	C	46	HIS
3	C	107	ASN

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Mol	Chain	Res	Type
3	C	331	GLN
4	D	49	ASN
4	D	132	GLN
4	D	140	ASN
4	D	197	GLN
4	D	231	HIS
4	D	263	HIS
5	E	83	GLN
5	E	102	ASN
5	E	153	ASN
5	E	167	GLN
6	F	17	GLN
6	F	28	GLN
6	F	125	GLN
6	F	137	HIS
7	G	61	ASN
7	G	65	ASN
7	G	96	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	ADP	A	501	-	22,29,29	1.39	3 (13%)	27,45,45	2.56	4 (14%)
9	ADP	B	395	-	22,29,29	1.40	3 (13%)	27,45,45	2.47	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	A	501	-	-	0/12/32/32	0/3/3/3
9	ADP	B	395	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	501	ADP	O4'-C1'	2.11	1.43	1.41
9	B	395	ADP	O4'-C1'	2.34	1.44	1.41
9	B	395	ADP	PB-O1B	3.13	1.61	1.51
9	A	501	ADP	PB-O1B	3.14	1.61	1.51
9	B	395	ADP	C2-N1	3.59	1.40	1.33
9	A	501	ADP	C2-N1	3.63	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	395	ADP	N3-C2-N1	-11.39	120.17	128.89
9	A	501	ADP	N3-C2-N1	-11.26	120.27	128.89
9	A	501	ADP	C4'-O4'-C1'	-4.19	105.12	109.72
9	A	501	ADP	PA-O3A-PB	-3.40	121.28	132.67
9	B	395	ADP	PA-O3A-PB	-2.76	123.40	132.67
9	A	501	ADP	C4-C5-N7	-2.62	107.07	109.48
9	B	395	ADP	C4-C5-N7	-2.30	107.37	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	501	ADP	2	0
9	B	395	ADP	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	397/418 (94%)	-0.24	8 (2%) 68 64	21, 48, 87, 109	0
2	B	203/394 (51%)	-0.08	6 (2%) 54 47	29, 62, 101, 113	0
3	C	341/372 (91%)	-0.30	3 (0%) 85 84	27, 44, 71, 92	0
4	D	283/300 (94%)	-0.35	1 (0%) 93 92	25, 42, 66, 92	0
5	E	173/178 (97%)	-0.09	6 (3%) 48 40	44, 60, 86, 99	0
6	F	167/168 (99%)	-0.49	0 100 100	25, 36, 48, 75	0
7	G	134/151 (88%)	0.06	2 (1%) 76 73	36, 67, 86, 94	0
All	All	1698/1981 (85%)	-0.24	26 (1%) 76 73	21, 47, 87, 113	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	211	ASP	4.8
2	B	174	SER	4.3
7	G	67	LYS	3.5
2	B	337	LEU	3.3
2	B	173	PHE	3.2
5	E	89	SER	3.2
5	E	154	ASP	2.9
1	A	360	PRO	2.9
1	A	359	LYS	2.9
3	C	127	GLN	2.7
5	E	151	PRO	2.7
2	B	340	PHE	2.5
7	G	19	TYR	2.4
1	A	68	GLU	2.4
5	E	153	ASN	2.3
1	A	352	GLU	2.3
1	A	39	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	368	ASP	2.2
2	B	183	ASP	2.2
5	E	175	GLY	2.2
1	A	362	PRO	2.2
1	A	415	GLY	2.2
3	C	367	LYS	2.2
1	A	416	VAL	2.2
2	B	184	ILE	2.1
5	E	86	ASN	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, 95^{th} 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(Å^2)	Q<0.9
9	ADP	A	501	27/27	0.88	0.17	-0.10	55,64,95,96	0
9	ADP	B	395	27/27	0.93	0.15	-0.20	54,60,74,76	0
8	CA	A	500	1/1	0.97	0.17	-	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.