



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:29 am BST

PDB ID : 2P9P  
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 : 2.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

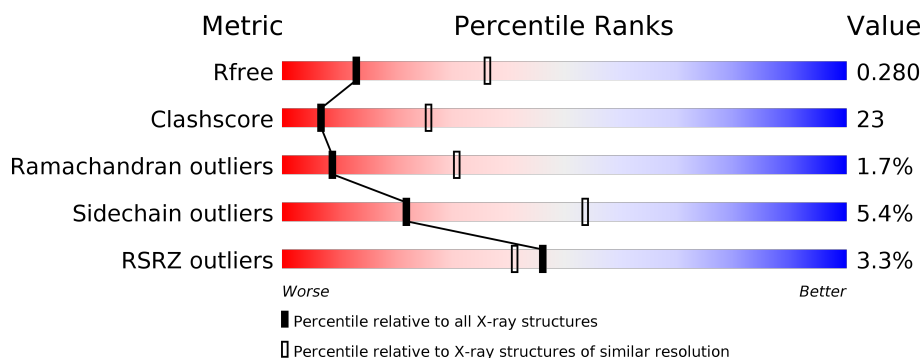
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>• 7%</div> </div> </div>
2	B	394	<div> <div>7%</div> <div> <div></div> <div>27%</div> <div>17%</div> <div>•</div> <div>53%</div> </div> </div>
3	C	372	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>• • 8%</div> </div> </div>
4	D	300	<div> <div></div> <div> <div></div> <div>59%</div> <div>31%</div> <div>• 9%</div> </div> </div>
5	E	178	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>5% • •</div> </div> </div>
6	F	168	<div> <div></div> <div> <div></div> <div>55%</div> <div>40%</div> <div>• • •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	G	151	<div><div></div><div>8%</div><div>44%</div><div>32%</div><div>9%</div><div>15%</div></div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13192 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	388	Total	C	N	O	S	0	0	0
			3078	1980	509	574	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1451	931	248	268	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	273	Total	C	N	O	S	0	0	0
			2213	1407	385	413	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1406	903	235	259	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	165	Total	C	N	O	S	0	0	0
			1359	868	237	245	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	128	Total	C	N	O	S	0	0	0
			982	619	173	187	3			

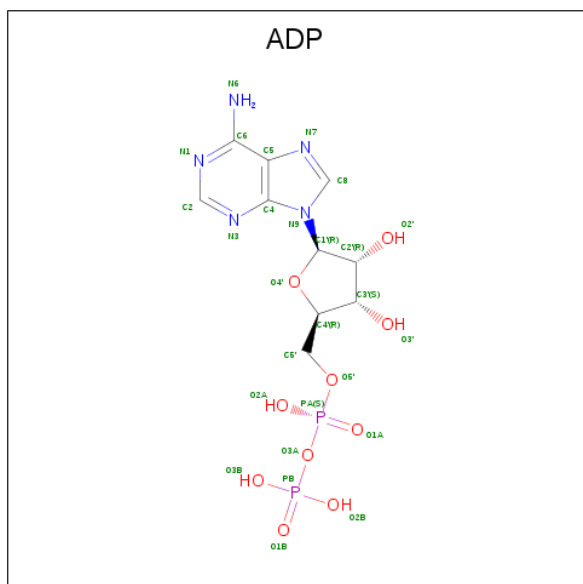
There are 2 discrepancies between the modelled and reference sequences:

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<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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		

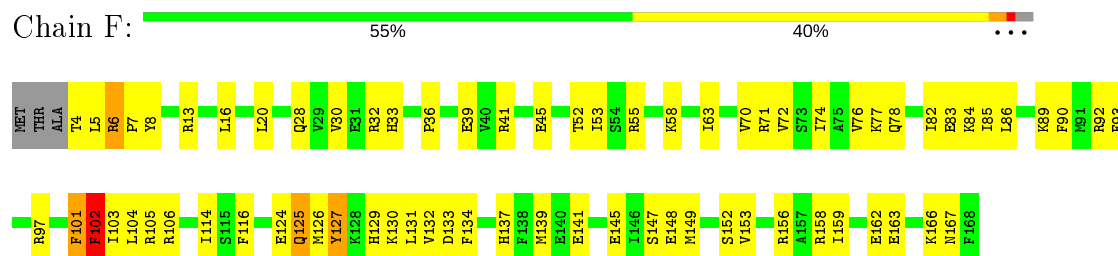


- Molecule 1: Actin-like protein 3

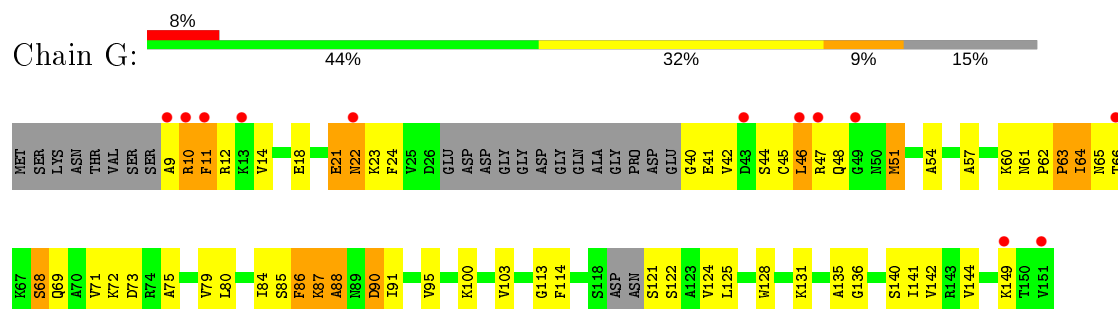




- Molecule 6: Actin-related protein 2/3 complex subunit 4



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.97Å 128.93Å 202.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 46.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.4 (50.00-2.90) 82.7 (46.02-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.234 , 0.288 0.226 , 0.280	Depositor DCC
$R_{free}$ test set	2896 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 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	0.47	0/3156	0.67	0/4287
2	B	0.43	0/1473	0.64	0/1986
3	C	0.44	0/2717	0.72	1/3688 (0.0%)
4	D	0.43	0/2261	0.64	0/3050
5	E	0.40	0/1440	0.69	0/1943
6	F	0.45	0/1381	0.66	0/1851
7	G	0.38	0/992	0.62	0/1331
All	All	0.44	0/13420	0.67	1/18136 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
5	E	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	283	GLY	N-CA-C	6.65	129.73	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	97	TYR	Sidechain
5	E	48	TYR	Sidechain

## 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	3078	0	2970	143	0
2	B	1451	0	1474	75	0
3	C	2648	0	2602	127	0
4	D	2213	0	2176	89	0
5	E	1406	0	1398	86	0
6	F	1359	0	1398	67	0
7	G	982	0	1012	58	0
8	A	1	0	0	0	0
9	A	27	0	12	3	0
9	B	27	0	12	2	0
All	All	13192	0	13054	607	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 23.

All (607) 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:282:GLY:HA3	3:C:370:LYS:HE3	1.34	1.08
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.41	0.99
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.46	0.97
6:F:130:LYS:HE2	6:F:130:LYS:HA	1.48	0.92
6:F:20:LEU:HD23	6:F:70:VAL:HG21	1.53	0.91
2:B:279:ALA:HB1	2:B:320:GLU:HG2	1.51	0.90
7:G:23:LYS:HG2	7:G:24:PHE:H	1.38	0.89
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.54	0.88
3:C:183:THR:HG22	3:C:184:PRO:HD2	1.57	0.87
6:F:163:GLU:HA	6:F:166:LYS:HE3	1.56	0.86
2:B:205:ASN:HD22	2:B:208:ALA:H	1.22	0.86
1:A:311:VAL:O	1:A:314:PRO:HD2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:ALA:HB3	5:E:135:GLN:HE22	1.41	0.85
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.58	0.85
2:B:279:ALA:CB	2:B:320:GLU:HG2	2.08	0.83
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.41	0.83
1:A:239:VAL:HG11	5:E:48:TYR:HD1	1.42	0.83
5:E:152:GLN:HB3	5:E:155:LYS:NZ	1.93	0.83
5:E:88:LYS:H	5:E:153:ASN:ND2	1.78	0.81
1:A:87:ASP:CG	4:D:264:THR:HG22	2.01	0.81
1:A:79:ARG:NE	1:A:79:ARG:HA	1.95	0.81
2:B:165:HIS:CD2	2:B:181:ARG:HG2	2.16	0.81
1:A:116:PRO:O	1:A:117:LEU:HB2	1.82	0.79
3:C:107:ASN:ND2	3:C:109:LYS:H	1.79	0.79
6:F:89:LYS:HG2	6:F:92:ARG:HH22	1.46	0.79
4:D:65:LYS:HA	4:D:65:LYS:HE2	1.62	0.79
1:A:309:ILE:HA	1:A:312:ARG:NE	1.98	0.78
2:B:158:ASP:HA	2:B:304:SER:O	1.82	0.78
5:E:152:GLN:HB3	5:E:155:LYS:HZ2	1.46	0.78
7:G:51:MET:HG3	7:G:87:LYS:HE2	1.63	0.77
4:D:189:ARG:NH2	4:D:197:GLN:HG3	2.01	0.76
3:C:183:THR:HG22	3:C:184:PRO:CD	2.13	0.76
5:E:95:MET:HG2	5:E:141:GLY:O	1.85	0.76
4:D:269:LYS:HE2	6:F:145:GLU:HB2	1.67	0.76
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.66	0.75
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.22	0.75
1:A:106:GLU:HG2	1:A:135:ASN:HB2	1.68	0.75
7:G:95:VAL:HG21	7:G:131:LYS:HB3	1.67	0.75
5:E:142:LEU:HD23	5:E:143:ARG:N	2.01	0.74
1:A:25:THR:HG22	1:A:26:GLU:HG2	1.69	0.74
1:A:289:ASN:HD22	1:A:290:PRO:N	1.85	0.74
1:A:246:ASP:OD1	5:E:50:LYS:HE3	1.87	0.74
3:C:96:ASN:O	3:C:97:ARG:HD3	1.87	0.74
3:C:10:PRO:HG2	6:F:124:GLU:HG2	1.68	0.73
3:C:201:SER:HB3	7:G:149:LYS:NZ	2.03	0.73
7:G:42:VAL:O	7:G:46:LEU:HB2	1.89	0.73
1:A:239:VAL:HG22	5:E:4:TYR:CZ	2.24	0.72
1:A:12:CYS:HB3	1:A:78:ILE:HD11	1.70	0.72
5:E:142:LEU:HD23	5:E:143:ARG:H	1.53	0.72
1:A:164:THR:HG23	1:A:181:ALA:HA	1.72	0.72
6:F:5:LEU:HD13	6:F:55:ARG:NH1	2.05	0.72
7:G:87:LYS:N	7:G:87:LYS:HD3	2.05	0.71
1:A:55:VAL:CG1	1:A:58:LEU:HD12	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:133:LEU:O	5:E:137:ARG:HG3	1.90	0.71
4:D:262:ILE:O	4:D:266:MET:HG3	1.90	0.71
2:B:290:ASP:HB2	2:B:293:THR:OG1	1.90	0.71
5:E:92:GLU:O	5:E:96:TYR:HD1	1.73	0.70
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.74	0.70
1:A:38:LYS:NZ	1:A:71:THR:OG1	2.25	0.69
2:B:290:ASP:O	2:B:294:ARG:HG3	1.92	0.69
5:E:152:GLN:O	5:E:155:LYS:HD2	1.91	0.69
1:A:4:ARG:CB	1:A:4:ARG:HH11	2.04	0.69
1:A:397:LYS:HE2	1:A:401:GLU:OE2	1.92	0.69
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.75	0.69
4:D:263:HIS:HB3	4:D:267:ARG:HH12	1.55	0.69
1:A:87:ASP:OD2	4:D:264:THR:HG22	1.93	0.69
3:C:173:ILE:HB	3:C:176:VAL:HG22	1.73	0.68
4:D:263:HIS:HB3	4:D:267:ARG:NH1	2.07	0.68
6:F:101:PHE:O	6:F:103:ILE:N	2.23	0.68
6:F:89:LYS:HA	6:F:92:ARG:HH12	1.56	0.68
5:E:10:ASP:HB3	5:E:12:ASP:OD1	1.93	0.68
4:D:202:HIS:HE1	4:D:218:ASP:O	1.77	0.67
2:B:282:LEU:HD23	2:B:321:LEU:HD11	1.75	0.67
4:D:282:PRO:O	4:D:283:ASP:HB2	1.93	0.67
3:C:284:ARG:NH1	3:C:286:ASP:O	2.28	0.67
1:A:120:PRO:HB3	1:A:409:ARG:HG2	1.76	0.67
6:F:53:ILE:HA	7:G:114:PHE:CD1	2.31	0.66
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.25	0.66
4:D:135:GLY:O	4:D:137:GLU:HG3	1.95	0.66
3:C:107:ASN:HD22	3:C:107:ASN:C	1.98	0.66
3:C:107:ASN:HD22	3:C:108:GLU:N	1.93	0.66
5:E:90:GLN:HG2	5:E:94:GLU:OE2	1.96	0.66
2:B:218:GLU:HG2	9:B:395:ADP:C5	2.31	0.65
1:A:19:LEU:HD13	1:A:96:VAL:HG13	1.75	0.65
5:E:87:SER:HA	5:E:153:ASN:OD1	1.97	0.65
1:A:164:THR:HA	1:A:180:VAL:O	1.96	0.65
3:C:168:ILE:HD11	3:C:217:VAL:HG11	1.79	0.65
3:C:222:HIS:C	3:C:224:SER:H	1.99	0.65
1:A:18:LYS:HD3	1:A:18:LYS:N	2.12	0.64
3:C:11:ILE:HG13	3:C:352:GLY:HA2	1.78	0.64
5:E:16:ILE:O	5:E:16:ILE:HG23	1.95	0.64
3:C:61:ALA:HB1	3:C:108:GLU:OE1	1.98	0.64
3:C:64:SER:O	3:C:66:ARG:HG3	1.97	0.64
4:D:129:PHE:HD2	4:D:237:ARG:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TYR:OH	1:A:103:ALA:HB2	1.98	0.64
5:E:32:ALA:HB3	5:E:135:GLN:NE2	2.13	0.64
1:A:55:VAL:HG23	6:F:159:ILE:HD12	1.81	0.63
7:G:51:MET:HG3	7:G:87:LYS:CE	2.27	0.63
2:B:236:GLU:HB3	6:F:105:ARG:NH1	2.13	0.63
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.80	0.63
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.12	0.63
1:A:140:TYR:CE2	1:A:142:ALA:HB2	2.34	0.63
2:B:254:VAL:HG13	2:B:257:GLU:HG2	1.80	0.63
3:C:201:SER:HB3	7:G:149:LYS:HZ1	1.62	0.63
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.34	0.62
1:A:14:THR:HG23	1:A:78:ILE:O	1.99	0.62
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.35	0.62
1:A:359:LYS:N	1:A:360:PRO:HD3	2.15	0.62
3:C:184:PRO:HB2	3:C:231:ALA:HB1	1.82	0.62
1:A:79:ARG:HB2	1:A:84:GLU:HG2	1.81	0.62
7:G:75:ALA:O	7:G:79:VAL:HG23	1.99	0.62
3:C:282:GLY:CA	3:C:370:LYS:HE3	2.19	0.62
6:F:89:LYS:HA	6:F:92:ARG:NH1	2.15	0.62
1:A:289:ASN:HD22	1:A:289:ASN:C	2.01	0.61
3:C:34:ILE:HB	3:C:46:HIS:HB2	1.81	0.61
5:E:44:GLU:HG2	5:E:48:TYR:CE2	2.36	0.61
1:A:311:VAL:C	1:A:314:PRO:HD2	2.19	0.61
5:E:153:ASN:OD1	5:E:154:ASP:N	2.33	0.61
1:A:12:CYS:HB3	1:A:78:ILE:CD1	2.30	0.61
3:C:173:ILE:O	3:C:177:GLU:HG2	2.00	0.61
3:C:347:THR:OG1	3:C:355:SER:HB2	2.01	0.61
5:E:30:GLY:HA3	5:E:135:GLN:OE1	2.00	0.61
1:A:113:THR:HB	1:A:144:GLN:HG3	1.82	0.61
4:D:61:LEU:HD23	4:D:63:PHE:CZ	2.35	0.61
5:E:146:GLU:O	5:E:146:GLU:HG2	1.99	0.61
3:C:173:ILE:HB	3:C:176:VAL:CG2	2.30	0.61
3:C:13:CYS:HA	3:C:331:GLN:NE2	2.16	0.60
7:G:87:LYS:N	7:G:87:LYS:CD	2.64	0.60
3:C:119:VAL:HG23	3:C:137:ILE:O	2.02	0.60
3:C:239:THR:HG22	3:C:240:LEU:N	2.15	0.60
3:C:60:TRP:HE1	3:C:65:ASN:ND2	1.98	0.60
5:E:86:ASN:O	5:E:87:SER:HB3	2.00	0.60
3:C:327:ASN:HB2	3:C:351:ASP:HB3	1.84	0.60
4:D:68:GLN:HA	4:D:72:ALA:HB3	1.84	0.60
2:B:342:ILE:HG22	2:B:342:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:66:THR:O	7:G:72:LYS:HE3	1.99	0.60
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.37	0.60
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.67	0.60
4:D:182:MET:HG3	4:D:200:PHE:CE1	2.37	0.60
4:D:203:ARG:HH11	4:D:203:ARG:HB3	1.65	0.60
1:A:234:VAL:HG22	1:A:279:PRO:HB2	1.83	0.60
1:A:289:ASN:ND2	1:A:291:ASP:H	2.00	0.60
3:C:13:CYS:HA	3:C:331:GLN:HE22	1.67	0.59
3:C:234:LYS:O	3:C:235:MET:HB2	2.02	0.59
4:D:37:ASP:HB3	4:D:41:VAL:HB	1.84	0.59
6:F:30:VAL:HG11	6:F:33:HIS:ND1	2.16	0.59
6:F:78:GLN:HG2	6:F:84:LYS:HA	1.84	0.59
6:F:20:LEU:HD23	6:F:70:VAL:CG2	2.29	0.59
4:D:180:VAL:HG11	6:F:153:VAL:HG12	1.85	0.59
2:B:343:ARG:HB2	2:B:343:ARG:NH1	2.17	0.59
3:C:212:ALA:HB3	3:C:255:GLU:OE2	2.02	0.59
1:A:249:GLY:O	1:A:251:LYS:N	2.36	0.58
1:A:343:VAL:HG13	1:A:363:ILE:HD11	1.86	0.58
1:A:4:ARG:HB2	1:A:4:ARG:HH11	1.68	0.58
1:A:61:PHE:CD2	1:A:69:LYS:HE3	2.38	0.58
1:A:30:ILE:HD13	1:A:375:TYR:CZ	2.38	0.58
5:E:50:LYS:NZ	5:E:159:TRP:O	2.37	0.58
1:A:172:ASP:O	1:A:198:ARG:HB2	2.04	0.58
1:A:55:VAL:HG12	1:A:58:LEU:HB2	1.85	0.58
1:A:76:TRP:O	1:A:79:ARG:HD2	2.03	0.58
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.39	0.58
1:A:55:VAL:O	1:A:55:VAL:HG12	2.04	0.58
2:B:330:LEU:O	2:B:331:LYS:HB2	2.04	0.58
4:D:203:ARG:NH1	4:D:203:ARG:HB3	2.19	0.58
3:C:144:THR:H	6:F:28:GLN:NE2	2.02	0.58
7:G:68:SER:OG	7:G:71:VAL:HG12	2.04	0.57
1:A:339:LEU:HD23	1:A:365:VAL:CG1	2.34	0.57
3:C:370:LYS:O	3:C:371:ILE:HB	2.04	0.57
7:G:51:MET:HB3	7:G:86:PHE:CE1	2.39	0.57
4:D:274:LEU:O	4:D:278:ASN:ND2	2.37	0.57
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.85	0.57
2:B:214:ARG:NH1	2:B:218:GLU:OE2	2.37	0.57
7:G:121:SER:O	7:G:124:VAL:HG12	2.05	0.57
2:B:165:HIS:HD2	2:B:181:ARG:HG2	1.63	0.57
1:A:393:VAL:HG21	1:A:414:PHE:CE2	2.40	0.57
3:C:224:SER:HB2	7:G:142:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:GLU:O	5:E:96:TYR:CD1	2.57	0.57
3:C:263:HIS:HD1	3:C:328:SER:HG	1.52	0.57
2:B:320:GLU:HA	2:B:323:GLN:HE21	1.69	0.56
1:A:140:TYR:HE2	1:A:142:ALA:HB2	1.70	0.56
7:G:80:LEU:O	7:G:84:ILE:HD13	2.05	0.56
1:A:309:ILE:HA	1:A:312:ARG:HE	1.68	0.56
7:G:23:LYS:HG2	7:G:24:PHE:N	2.14	0.56
1:A:194:PRO:C	1:A:195:ILE:HD12	2.26	0.56
2:B:335:GLU:O	2:B:337:LEU:N	2.38	0.56
4:D:146:TYR:OH	4:D:248:ARG:HG3	2.05	0.56
5:E:130:ARG:HG3	5:E:130:ARG:HH11	1.70	0.56
4:D:182:MET:HG3	4:D:200:PHE:CD1	2.41	0.56
5:E:150:ASP:C	5:E:152:GLN:H	2.09	0.56
3:C:50:GLU:OE1	3:C:88:PRO:HG3	2.06	0.56
5:E:112:PRO:O	5:E:113:LEU:HB2	2.06	0.56
6:F:130:LYS:CE	6:F:130:LYS:HA	2.30	0.56
5:E:40:ASP:O	5:E:43:ASP:HB2	2.06	0.55
7:G:62:PRO:C	7:G:64:ILE:H	2.09	0.55
1:A:190:ILE:HG22	1:A:191:LYS:N	2.20	0.55
3:C:216:ARG:NH1	3:C:255:GLU:O	2.39	0.55
6:F:4:THR:HG23	6:F:55:ARG:HE	1.71	0.55
3:C:173:ILE:HG22	3:C:175:GLU:HG3	1.89	0.55
1:A:87:ASP:OD2	4:D:267:ARG:HD2	2.06	0.55
3:C:144:THR:O	3:C:161:SER:HB2	2.07	0.55
3:C:14:HIS:HA	3:C:24:ALA:O	2.05	0.55
4:D:137:GLU:OE2	4:D:158:LYS:HE2	2.05	0.55
2:B:238:THR:HG22	6:F:106:ARG:CZ	2.37	0.55
2:B:322:LYS:HG2	2:B:340:PHE:HZ	1.72	0.55
5:E:150:ASP:O	5:E:152:GLN:N	2.40	0.55
3:C:179:ARG:HH11	3:C:179:ARG:HG3	1.72	0.55
6:F:5:LEU:HD13	6:F:55:ARG:HH12	1.71	0.55
6:F:85:ILE:C	6:F:85:ILE:HD12	2.27	0.55
3:C:47:GLU:OE2	3:C:49:LYS:NZ	2.40	0.55
4:D:164:VAL:HG22	4:D:224:THR:OG1	2.07	0.55
1:A:55:VAL:HG13	1:A:58:LEU:HD12	1.88	0.54
3:C:358:ASP:HB3	3:C:361:SER:HB2	1.90	0.54
3:C:119:VAL:HB	3:C:138:LYS:HD3	1.89	0.54
1:A:91:ARG:O	1:A:94:GLU:HB2	2.07	0.54
2:B:236:GLU:HB3	6:F:105:ARG:HH12	1.72	0.54
2:B:314:PRO:O	2:B:318:GLU:HG3	2.07	0.54
6:F:158:ARG:O	6:F:162:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ARG:CB	2:B:281:LEU:HD21	2.37	0.54
3:C:193:GLU:HB3	3:C:195:MET:HE2	1.89	0.54
3:C:16:TRP:CZ2	3:C:23:ILE:HD12	2.43	0.54
3:C:239:THR:HG22	3:C:240:LEU:H	1.73	0.54
3:C:250:VAL:HG23	3:C:260:ALA:HB2	1.88	0.54
4:D:281:ARG:C	4:D:283:ASP:H	2.11	0.54
3:C:140:PRO:HG2	3:C:167:ARG:HE	1.73	0.54
3:C:72:THR:HA	3:C:98:ALA:HB1	1.90	0.54
3:C:7:LEU:HD23	3:C:7:LEU:N	2.23	0.54
5:E:76:SER:O	5:E:80:LYS:HD3	2.08	0.54
3:C:131:TRP:O	3:C:131:TRP:HE3	1.90	0.53
3:C:268:VAL:HA	3:C:284:ARG:H	1.72	0.53
2:B:298:TYR:O	2:B:340:PHE:HB2	2.08	0.53
3:C:201:SER:HB3	7:G:149:LYS:HZ2	1.74	0.53
6:F:145:GLU:O	6:F:149:MET:HG3	2.09	0.53
3:C:29:ASN:OD1	3:C:31:GLU:N	2.41	0.53
4:D:199:LEU:HD12	4:D:199:LEU:N	2.24	0.53
5:E:140:THR:O	5:E:144:LEU:HB2	2.09	0.53
5:E:112:PRO:HB2	5:E:171:LYS:HD2	1.91	0.53
3:C:7:LEU:HD13	3:C:27:PRO:HB2	1.91	0.53
4:D:30:ALA:HB2	4:D:52:LYS:HD3	1.91	0.53
5:E:105:ILE:HD13	5:E:130:ARG:NH1	2.23	0.53
5:E:150:ASP:C	5:E:152:GLN:N	2.60	0.53
7:G:103:VAL:HG11	7:G:136:GLY:HA3	1.90	0.53
3:C:155:VAL:HG11	3:C:180:PRO:HG2	1.90	0.53
3:C:229:ALA:HB2	3:C:237:VAL:HG22	1.91	0.53
6:F:53:ILE:N	6:F:53:ILE:HD12	2.23	0.53
6:F:58:LYS:HA	6:F:58:LYS:HE2	1.90	0.53
1:A:283:PHE:C	1:A:285:PRO:HD3	2.29	0.53
6:F:163:GLU:O	6:F:167:ASN:ND2	2.42	0.53
6:F:71:ARG:HA	6:F:116:PHE:O	2.08	0.53
4:D:74:GLU:N	4:D:74:GLU:OE1	2.27	0.53
1:A:128:GLU:O	1:A:132:GLU:HB2	2.08	0.52
1:A:328:PHE:CZ	9:A:501:ADP:H2	2.27	0.52
3:C:126:GLU:CB	3:C:131:TRP:HZ3	2.19	0.52
4:D:248:ARG:HD3	4:D:248:ARG:O	2.09	0.52
3:C:102:VAL:HA	3:C:112:ALA:O	2.08	0.52
1:A:39:GLU:HG3	1:A:39:GLU:O	2.08	0.52
6:F:97:ARG:HH11	6:F:97:ARG:HG3	1.73	0.52
1:A:111:LEU:HD23	1:A:111:LEU:C	2.29	0.52
1:A:151:ALA:O	1:A:154:THR:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ASP:O	3:C:235:MET:N	2.42	0.52
4:D:67:LEU:HD23	4:D:144:ILE:HD12	1.92	0.52
5:E:40:ASP:CG	5:E:143:ARG:HH12	2.13	0.52
5:E:88:LYS:N	5:E:153:ASN:ND2	2.55	0.52
5:E:44:GLU:HG2	5:E:48:TYR:HE2	1.75	0.52
1:A:343:VAL:O	1:A:347:LEU:HD13	2.10	0.52
4:D:35:PHE:N	4:D:35:PHE:CD2	2.78	0.52
5:E:146:GLU:OE2	5:E:147:LYS:HG2	2.10	0.52
1:A:79:ARG:HB2	1:A:84:GLU:CG	2.39	0.51
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.92	0.51
1:A:258:GLY:C	1:A:259:ILE:HD12	2.31	0.51
5:E:82:LEU:HD23	5:E:148:VAL:HG21	1.93	0.51
7:G:149:LYS:N	7:G:149:LYS:HD3	2.25	0.51
3:C:189:MET:HA	3:C:195:MET:HE1	1.93	0.51
1:A:173:GLY:O	1:A:174:VAL:HG23	2.10	0.51
1:A:174:VAL:CG1	1:A:175:THR:N	2.73	0.51
1:A:90:GLU:HG3	1:A:129:ILE:HG23	1.93	0.51
7:G:113:GLY:HA3	7:G:125:LEU:HD11	1.91	0.51
2:B:161:ASP:O	2:B:187:ARG:HG3	2.11	0.51
4:D:281:ARG:HG3	4:D:281:ARG:HH11	1.76	0.51
7:G:91:ILE:HG22	7:G:131:LYS:HG2	1.92	0.51
2:B:320:GLU:HA	2:B:323:GLN:NE2	2.26	0.51
1:A:237:ASP:OD2	1:A:239:VAL:HG23	2.11	0.51
2:B:182:LEU:HG	2:B:281:LEU:CD1	2.40	0.51
3:C:64:SER:O	3:C:66:ARG:N	2.44	0.51
4:D:203:ARG:HG2	4:D:203:ARG:O	2.10	0.51
6:F:76:VAL:HG12	6:F:77:LYS:N	2.26	0.51
3:C:44:GLN:NE2	3:C:47:GLU:HG3	2.26	0.51
1:A:279:PRO:HG3	1:A:328:PHE:CE1	2.46	0.51
2:B:334:VAL:HG12	2:B:334:VAL:O	2.11	0.51
6:F:8:TYR:CD1	6:F:55:ARG:HB2	2.46	0.51
1:A:171:GLY:HA3	9:A:501:ADP:O3A	2.11	0.50
1:A:406:SER:O	1:A:409:ARG:HB2	2.12	0.50
5:E:88:LYS:N	5:E:153:ASN:HD21	2.09	0.50
1:A:284:HIS:NE2	5:E:2:PRO:HA	2.27	0.50
6:F:53:ILE:HG23	7:G:114:PHE:CE1	2.47	0.50
3:C:131:TRP:O	3:C:131:TRP:CE3	2.64	0.50
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.51	0.50
2:B:299:LYS:O	2:B:300:HIS:ND1	2.44	0.50
3:C:14:HIS:N	3:C:331:GLN:HE22	2.09	0.50
7:G:140:SER:O	7:G:144:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ASN:ND2	3:C:22:GLN:HB2	2.27	0.50
3:C:21:THR:HG22	3:C:22:GLN:HG3	1.93	0.50
4:D:229:PRO:O	4:D:233:ASN:HB3	2.12	0.50
7:G:11:PHE:O	7:G:14:VAL:HG12	2.12	0.50
2:B:214:ARG:HG2	2:B:214:ARG:HH11	1.76	0.50
4:D:32:GLU:OE2	4:D:44:HIS:NE2	2.39	0.50
1:A:61:PHE:C	1:A:66:ALA:HB2	2.33	0.50
1:A:69:LYS:HB3	1:A:72:TYR:CD1	2.47	0.50
3:C:269:LEU:H	3:C:283:GLY:HA3	1.77	0.50
2:B:277:GLY:O	2:B:279:ALA:N	2.44	0.49
1:A:205:GLN:HE22	1:A:221:LEU:HG	1.77	0.49
2:B:217:LYS:O	2:B:221:CYS:HB2	2.12	0.49
7:G:46:LEU:C	7:G:48:GLN:H	2.16	0.49
7:G:62:PRO:O	7:G:64:ILE:N	2.36	0.49
7:G:64:ILE:HG22	7:G:65:ASN:ND2	2.27	0.49
3:C:142:ARG:HH11	3:C:142:ARG:HG3	1.78	0.49
4:D:282:PRO:O	4:D:283:ASP:CB	2.61	0.49
4:D:67:LEU:HD13	4:D:120:CYS:O	2.13	0.49
5:E:150:ASP:OD1	5:E:151:PRO:HD2	2.11	0.49
3:C:283:GLY:O	3:C:284:ARG:HB2	2.11	0.49
4:D:158:LYS:HG3	4:D:159:ASP:OD1	2.12	0.49
1:A:169:ASP:O	1:A:175:THR:HG23	2.13	0.49
3:C:269:LEU:H	3:C:283:GLY:CA	2.25	0.49
3:C:31:GLU:HG2	3:C:49:LYS:HG2	1.95	0.49
4:D:244:ILE:HG23	4:D:245:HIS:N	2.27	0.49
6:F:30:VAL:HG11	6:F:33:HIS:CE1	2.48	0.49
3:C:172:TYR:CD2	3:C:172:TYR:C	2.86	0.49
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.43	0.49
2:B:237:THR:HG22	6:F:105:ARG:HG3	1.93	0.49
6:F:74:ILE:HD13	6:F:139:MET:HG2	1.94	0.49
2:B:335:GLU:O	2:B:336:LYS:C	2.49	0.49
4:D:67:LEU:O	4:D:72:ALA:HB2	2.13	0.49
7:G:54:ALA:O	7:G:57:ALA:HB3	2.13	0.49
1:A:309:ILE:O	1:A:312:ARG:HG3	2.14	0.48
2:B:331:LYS:O	2:B:331:LYS:HD3	2.13	0.48
4:D:198:VAL:HA	4:D:224:THR:O	2.12	0.48
7:G:141:ILE:O	7:G:144:VAL:N	2.43	0.48
1:A:4:ARG:HD3	1:A:5:LEU:HG	1.96	0.48
1:A:61:PHE:CE2	1:A:69:LYS:HE3	2.47	0.48
2:B:182:LEU:HD11	2:B:278:VAL:N	2.28	0.48
5:E:134:GLN:O	5:E:138:GLN:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HA	1:A:196:ALA:HB2	1.94	0.48
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.95	0.48
4:D:189:ARG:CZ	4:D:197:GLN:HG3	2.43	0.48
5:E:152:GLN:HB3	5:E:155:LYS:HZ3	1.74	0.48
7:G:69:GLN:O	7:G:73:ASP:OD1	2.32	0.48
4:D:202:HIS:CE1	4:D:218:ASP:O	2.63	0.48
5:E:60:ILE:HD12	5:E:116:ILE:CG2	2.43	0.48
7:G:87:LYS:O	7:G:90:ASP:N	2.39	0.48
1:A:71:THR:OG1	1:A:71:THR:O	2.31	0.48
2:B:159:SER:HB2	2:B:164:THR:HG23	1.94	0.48
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.44	0.48
2:B:221:CYS:HA	2:B:258:ARG:O	2.14	0.48
5:E:113:LEU:C	5:E:115:ALA:H	2.17	0.48
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.43	0.48
4:D:244:ILE:CG2	4:D:245:HIS:N	2.77	0.48
1:A:135:ASN:ND2	4:D:256:LYS:HE3	2.29	0.48
3:C:10:PRO:CG	6:F:124:GLU:HG2	2.42	0.48
1:A:140:TYR:CE1	1:A:411:ASN:HB3	2.49	0.48
4:D:198:VAL:C	4:D:199:LEU:HD12	2.34	0.48
7:G:100:LYS:NZ	7:G:135:ALA:O	2.47	0.48
3:C:189:MET:HA	3:C:195:MET:CE	2.43	0.47
3:C:27:PRO:HG3	3:C:33:HIS:CD2	2.49	0.47
5:E:152:GLN:OE1	5:E:152:GLN:HA	2.14	0.47
2:B:198:LEU:C	2:B:200:ARG:N	2.66	0.47
3:C:14:HIS:H	3:C:331:GLN:HE22	1.62	0.47
3:C:337:GLY:HA3	3:C:342:CYS:HA	1.95	0.47
3:C:63:ASP:C	3:C:65:ASN:H	2.16	0.47
6:F:153:VAL:O	6:F:156:ARG:HG2	2.14	0.47
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.34	0.47
3:C:178:GLU:O	3:C:179:ARG:C	2.52	0.47
3:C:52:ASN:N	3:C:73:ASP:OD2	2.44	0.47
4:D:248:ARG:C	4:D:248:ARG:HD3	2.34	0.47
4:D:2:ILE:HG21	6:F:163:GLU:HG2	1.96	0.47
3:C:27:PRO:HG2	3:C:29:ASN:HB2	1.97	0.47
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.96	0.47
3:C:96:ASN:C	3:C:97:ARG:HD3	2.35	0.47
5:E:18:ASN:ND2	5:E:66:ARG:NE	2.63	0.47
2:B:331:LYS:C	2:B:331:LYS:HD3	2.35	0.47
5:E:60:ILE:HD12	5:E:116:ILE:HG23	1.97	0.47
1:A:152:SER:C	1:A:154:THR:N	2.68	0.47
4:D:251:LEU:O	4:D:255:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:HG13	1:A:163:LEU:HD22	1.97	0.47
1:A:149:LEU:HD11	1:A:180:VAL:HB	1.96	0.47
1:A:69:LYS:HB3	1:A:72:TYR:HD1	1.80	0.47
1:A:189:CYS:O	1:A:303:VAL:HG13	2.15	0.47
1:A:85:ASP:OD2	1:A:88:LEU:HD22	2.14	0.47
2:B:163:VAL:HG23	2:B:182:LEU:O	2.15	0.47
4:D:53:THR:C	4:D:54:LYS:HD2	2.34	0.47
7:G:87:LYS:O	7:G:88:ALA:C	2.54	0.47
1:A:174:VAL:HG12	1:A:175:THR:N	2.30	0.46
2:B:184:ILE:HG13	2:B:265:LEU:HD23	1.96	0.46
3:C:122:ILE:O	3:C:134:CYS:HA	2.15	0.46
1:A:152:SER:C	1:A:154:THR:H	2.18	0.46
1:A:216:PRO:HB2	1:A:219:GLN:HB2	1.97	0.46
2:B:197:LEU:O	2:B:202:TYR:HB2	2.16	0.46
4:D:270:THR:HG1	6:F:93:PHE:HE2	1.64	0.46
7:G:44:SER:OG	7:G:48:GLN:NE2	2.48	0.46
2:B:261:ALA:HB3	2:B:262:PRO:CD	2.37	0.46
4:D:48:PRO:HB3	4:D:56:MET:HE3	1.96	0.46
5:E:58:TYR:CD1	5:E:168:PHE:HZ	2.33	0.46
1:A:112:LEU:HD11	1:A:130:MET:CE	2.44	0.46
1:A:257:THR:HG22	1:A:268:SER:HB3	1.97	0.46
4:D:66:GLU:OE1	4:D:144:ILE:HA	2.15	0.46
2:B:198:LEU:C	2:B:200:ARG:H	2.19	0.46
3:C:230:ASP:OD2	3:C:272:TYR:OH	2.29	0.46
7:G:51:MET:O	7:G:54:ALA:HB3	2.16	0.46
2:B:323:GLN:HB3	7:G:11:PHE:HD1	1.80	0.46
3:C:335:LEU:HA	3:C:335:LEU:HD23	1.76	0.46
7:G:51:MET:HB3	7:G:86:PHE:CZ	2.49	0.46
1:A:190:ILE:O	1:A:191:LYS:HD3	2.16	0.46
1:A:327:MET:HG3	1:A:374:ARG:NH1	2.31	0.46
4:D:140:ASN:HD22	4:D:140:ASN:N	2.14	0.46
7:G:103:VAL:HG11	7:G:136:GLY:CA	2.45	0.46
1:A:389:GLU:CD	1:A:414:PHE:HB2	2.37	0.45
2:B:302:VAL:HG13	2:B:302:VAL:O	2.16	0.45
3:C:13:CYS:CA	3:C:331:GLN:HE22	2.29	0.45
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.97	0.45
4:D:153:TYR:CD1	4:D:153:TYR:N	2.85	0.45
5:E:139:GLU:O	5:E:143:ARG:HB2	2.16	0.45
6:F:20:LEU:HD12	6:F:132:VAL:HG23	1.99	0.45
3:C:107:ASN:ND2	3:C:107:ASN:C	2.64	0.45
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:51:MET:HG3	7:G:87:LYS:NZ	2.31	0.45
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.52	0.45
2:B:157:VAL:HB	2:B:303:LEU:CD1	2.47	0.45
4:D:129:PHE:CD2	4:D:237:ARG:HG3	2.48	0.45
5:E:73:LEU:HD23	5:E:168:PHE:HB3	1.98	0.45
5:E:87:SER:OG	5:E:90:GLN:HB2	2.17	0.45
7:G:84:ILE:C	7:G:86:PHE:H	2.20	0.45
2:B:322:LYS:HG2	2:B:340:PHE:CZ	2.51	0.45
4:D:281:ARG:C	4:D:283:ASP:N	2.69	0.45
1:A:219:GLN:HB3	1:A:222:GLU:OE1	2.16	0.45
1:A:260:ASN:O	1:A:264:LYS:HA	2.17	0.45
5:E:15:LEU:HD22	5:E:63:GLU:HG3	1.99	0.45
5:E:60:ILE:HD13	5:E:66:ARG:HG2	1.98	0.45
3:C:253:ILE:O	3:C:254:THR:HG23	2.16	0.45
6:F:130:LYS:CA	6:F:130:LYS:HE2	2.29	0.45
6:F:126:MET:CE	6:F:131:LEU:HD21	2.47	0.45
2:B:323:GLN:HB3	7:G:11:PHE:O	2.17	0.45
3:C:219:TRP:CE2	3:C:227:CYS:HB2	2.51	0.44
3:C:184:PRO:HB2	3:C:231:ALA:CB	2.46	0.44
1:A:289:ASN:HA	1:A:290:PRO:HD3	1.78	0.44
3:C:371:ILE:O	3:C:372:VAL:HB	2.18	0.44
5:E:156:PRO:O	5:E:157:SER:C	2.55	0.44
7:G:87:LYS:H	7:G:87:LYS:CE	2.30	0.44
2:B:217:LYS:HE2	2:B:217:LYS:HB3	1.86	0.44
2:B:223:VAL:HG23	2:B:310:TYR:HB3	1.99	0.44
4:D:151:THR:HG22	4:D:152:MET:N	2.33	0.44
7:G:41:GLU:O	7:G:44:SER:HB3	2.17	0.44
4:D:202:HIS:C	4:D:204:GLU:H	2.20	0.44
4:D:38:PHE:O	4:D:41:VAL:HG23	2.16	0.44
5:E:95:MET:HG2	5:E:141:GLY:C	2.38	0.44
2:B:157:VAL:HB	2:B:303:LEU:HD13	1.99	0.44
3:C:33:HIS:ND1	3:C:47:GLU:HG2	2.32	0.44
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.53	0.44
7:G:63:PRO:O	7:G:72:LYS:HE2	2.18	0.44
2:B:310:TYR:CE1	9:B:395:ADP:H2	2.35	0.44
4:D:77:LYS:HA	4:D:84:LEU:HD12	2.00	0.44
3:C:153:ASN:OD1	3:C:155:VAL:N	2.41	0.44
5:E:112:PRO:O	5:E:113:LEU:CB	2.63	0.44
3:C:222:HIS:C	3:C:224:SER:N	2.67	0.43
4:D:169:PHE:HB2	4:D:175:VAL:HG22	1.99	0.43
4:D:266:MET:SD	6:F:90:PHE:HA	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:THR:C	3:C:74:ARG:H	2.20	0.43
4:D:171:ASP:OD2	4:D:173:ASP:HB2	2.18	0.43
1:A:205:GLN:NE2	1:A:221:LEU:HG	2.33	0.43
1:A:239:VAL:HG22	5:E:4:TYR:OH	2.17	0.43
1:A:343:VAL:HG11	1:A:363:ILE:HG13	2.00	0.43
6:F:125:GLN:O	6:F:126:MET:HG2	2.18	0.43
2:B:225:TYR:CE2	2:B:319:ARG:HD2	2.53	0.43
3:C:167:ARG:HD2	3:C:169:PHE:CZ	2.54	0.43
4:D:173:ASP:OD2	6:F:89:LYS:HE2	2.18	0.43
4:D:223:ILE:HD12	4:D:223:ILE:N	2.33	0.43
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.53	0.43
5:E:113:LEU:C	5:E:115:ALA:N	2.71	0.43
2:B:254:VAL:HG12	2:B:258:ARG:HG3	1.99	0.43
4:D:2:ILE:O	4:D:250:TYR:HE1	2.01	0.43
6:F:52:THR:HG22	6:F:53:ILE:N	2.33	0.43
1:A:19:LEU:HD23	1:A:19:LEU:N	2.33	0.43
3:C:170:SER:HB2	3:C:195:MET:CE	2.49	0.43
3:C:252:PHE:CZ	3:C:258:LEU:HD21	2.54	0.43
1:A:216:PRO:O	1:A:217:PRO:C	2.56	0.43
1:A:299:VAL:O	1:A:303:VAL:HG23	2.18	0.43
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.49	0.43
2:B:163:VAL:HG13	2:B:165:HIS:CE1	2.53	0.43
3:C:173:ILE:CG2	3:C:175:GLU:HG3	2.49	0.43
3:C:170:SER:HB2	3:C:195:MET:HE3	2.01	0.43
1:A:321:LEU:HD12	1:A:369:THR:HG22	1.99	0.43
1:A:4:ARG:NH1	1:A:4:ARG:CG	2.78	0.43
3:C:79:TRP:CH2	3:C:88:PRO:HB3	2.54	0.43
4:D:102:LEU:HB3	4:D:103:PRO:HD2	2.00	0.43
3:C:119:VAL:HG21	3:C:136:HIS:HB3	2.01	0.43
5:E:58:TYR:OH	5:E:68:LEU:HD23	2.18	0.43
5:E:86:ASN:O	5:E:87:SER:CB	2.67	0.43
2:B:343:ARG:HH11	2:B:343:ARG:HB2	1.84	0.43
7:G:10:ARG:O	7:G:12:ARG:N	2.52	0.43
1:A:117:LEU:HD13	1:A:190:ILE:HD12	2.00	0.42
1:A:169:ASP:HA	1:A:322:SER:O	2.18	0.42
3:C:223:ASP:C	3:C:223:ASP:OD1	2.57	0.42
7:G:40:GLY:O	7:G:44:SER:N	2.52	0.42
1:A:285:PRO:HG2	1:A:294:GLN:O	2.19	0.42
2:B:202:TYR:CZ	2:B:252:ILE:HB	2.54	0.42
2:B:335:GLU:O	2:B:338:SER:N	2.42	0.42
4:D:59:ILE:HD13	4:D:61:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:TYR:HB3	4:D:92:ASN:ND2	2.34	0.42
1:A:308:PRO:O	1:A:311:VAL:HG12	2.19	0.42
1:A:397:LYS:O	1:A:400:TYR:HB3	2.19	0.42
5:E:50:LYS:HG2	5:E:163:PHE:CZ	2.54	0.42
6:F:104:LEU:HD21	6:F:114:ILE:HD11	2.01	0.42
6:F:72:VAL:HB	6:F:116:PHE:HB2	2.02	0.42
1:A:339:LEU:HD23	1:A:365:VAL:HG13	2.01	0.42
5:E:144:LEU:HD22	5:E:144:LEU:O	2.19	0.42
6:F:101:PHE:CG	6:F:104:LEU:HD12	2.54	0.42
1:A:190:ILE:CG2	1:A:191:LYS:N	2.81	0.42
5:E:134:GLN:HG2	5:E:134:GLN:O	2.20	0.42
7:G:87:LYS:H	7:G:87:LYS:CD	2.33	0.42
1:A:61:PHE:O	1:A:66:ALA:HB2	2.19	0.42
3:C:239:THR:CG2	3:C:240:LEU:N	2.82	0.42
4:D:145:HIS:C	4:D:147:ARG:H	2.23	0.42
4:D:277:LEU:HD13	6:F:102:PHE:CE1	2.54	0.42
5:E:87:SER:HA	5:E:154:ASP:H	1.85	0.42
5:E:87:SER:HB2	5:E:153:ASN:HD21	1.85	0.42
6:F:127:TYR:O	6:F:130:LYS:N	2.53	0.42
7:G:23:LYS:CG	7:G:24:PHE:H	2.18	0.42
5:E:97:THR:O	5:E:101:THR:HG23	2.19	0.42
1:A:283:PHE:O	1:A:295:PRO:HB3	2.19	0.42
1:A:77:PRO:HG3	1:A:88:LEU:HB3	2.01	0.42
3:C:32:VAL:HB	3:C:48:LEU:HB2	2.02	0.42
4:D:59:ILE:HG22	4:D:93:VAL:HB	2.02	0.42
5:E:105:ILE:CD1	5:E:130:ARG:NH1	2.83	0.42
6:F:6:ARG:N	6:F:7:PRO:CD	2.83	0.42
5:E:130:ARG:NH1	5:E:130:ARG:HG3	2.35	0.42
1:A:15:GLY:O	1:A:16:TYR:CD2	2.73	0.42
1:A:298:GLU:O	1:A:301:ASP:HB3	2.20	0.42
1:A:38:LYS:HE2	1:A:72:TYR:CE2	2.55	0.42
4:D:130:GLN:OE1	4:D:130:GLN:HA	2.20	0.42
4:D:267:ARG:HH11	4:D:267:ARG:HG3	1.84	0.42
5:E:29:LYS:O	5:E:135:GLN:HG3	2.20	0.42
6:F:16:LEU:HD23	6:F:63:ILE:HD13	2.02	0.42
1:A:286:GLU:HB3	1:A:293:THR:HG22	2.02	0.41
3:C:110:LYS:HG2	3:C:124:TYR:HB3	2.01	0.41
1:A:289:ASN:HD22	1:A:290:PRO:CD	2.32	0.41
1:A:339:LEU:HD23	1:A:365:VAL:HG11	1.99	0.41
2:B:205:ASN:HD21	2:B:207:SER:HB2	1.85	0.41
5:E:56:LYS:HE3	5:E:170:ASN:OD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:ASN:HB3	5:E:154:ASP:OD2	2.20	0.41
1:A:278:GLY:O	1:A:281:ILE:HG12	2.20	0.41
1:A:327:MET:HG3	1:A:374:ARG:CZ	2.51	0.41
1:A:14:THR:HA	1:A:78:ILE:CG2	2.50	0.41
3:C:174:LYS:HB3	3:C:174:LYS:HE2	1.64	0.41
3:C:321:LEU:HD13	6:F:129:HIS:CE1	2.55	0.41
4:D:77:LYS:HD2	4:D:77:LYS:HA	1.79	0.41
4:D:265:ARG:NH2	6:F:148:GLU:HB3	2.34	0.41
6:F:86:LEU:HD22	6:F:149:MET:CE	2.51	0.41
1:A:229:GLU:HG2	9:A:501:ADP:C5	2.55	0.41
2:B:254:VAL:CG1	2:B:257:GLU:HG2	2.48	0.41
6:F:137:HIS:O	6:F:141:GLU:HG2	2.21	0.41
4:D:255:ILE:O	4:D:258:SER:HB3	2.21	0.41
5:E:144:LEU:HD22	5:E:148:VAL:HG23	2.02	0.41
5:E:153:ASN:CG	5:E:154:ASP:N	2.74	0.41
6:F:4:THR:HG23	6:F:55:ARG:NE	2.35	0.41
7:G:46:LEU:HD21	7:G:85:SER:CB	2.51	0.41
1:A:97:ILE:CG2	1:A:105:PRO:HD3	2.51	0.41
4:D:159:ASP:O	4:D:229:PRO:HD3	2.21	0.41
5:E:30:GLY:C	5:E:32:ALA:H	2.24	0.41
2:B:254:VAL:HG13	2:B:257:GLU:CG	2.50	0.41
7:G:21:GLU:O	7:G:22:ASN:ND2	2.54	0.41
1:A:108:HIS:O	1:A:137:PRO:HD2	2.20	0.41
1:A:235:CYS:O	1:A:334:ARG:NH1	2.54	0.41
1:A:4:ARG:HB2	1:A:4:ARG:NH1	2.35	0.41
3:C:77:TYR:CE2	3:C:90:LEU:HG	2.56	0.41
4:D:118:ARG:HD3	4:D:118:ARG:C	2.41	0.41
1:A:155:SER:HB2	1:A:370:HIS:HB3	2.02	0.41
4:D:31:VAL:N	4:D:47:ASN:OD1	2.42	0.41
7:G:86:PHE:CG	7:G:128:TRP:HZ2	2.39	0.41
2:B:202:TYR:CE1	2:B:252:ILE:HG22	2.56	0.41
2:B:295:SER:O	2:B:299:LYS:HG2	2.21	0.41
3:C:7:LEU:HG	3:C:9:GLU:O	2.20	0.41
5:E:42:VAL:O	5:E:46:ILE:HG13	2.21	0.41
1:A:259:ILE:N	1:A:259:ILE:HD12	2.36	0.41
1:A:307:CYS:HB3	1:A:308:PRO:HD2	2.03	0.41
2:B:163:VAL:HG22	2:B:164:THR:N	2.36	0.41
3:C:360:ARG:CG	3:C:361:SER:N	2.84	0.41
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.85	0.41
2:B:283:PHE:HE2	2:B:328:ARG:HD2	1.87	0.40
3:C:107:ASN:HD22	3:C:109:LYS:H	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:152:GLN:O	5:E:155:LYS:HB2	2.21	0.40
6:F:149:MET:HB2	6:F:149:MET:HE3	1.98	0.40
6:F:82:ILE:HG23	6:F:83:GLU:N	2.34	0.40
1:A:226:ALA:O	1:A:230:ARG:HB2	2.21	0.40
3:C:118:ARG:O	3:C:138:LYS:HD2	2.20	0.40
3:C:363:GLU:OE2	3:C:371:ILE:HD12	2.21	0.40
4:D:54:LYS:HE3	4:D:98:ASP:OD2	2.21	0.40
6:F:13:ARG:NH1	6:F:133:ASP:OD1	2.33	0.40
1:A:79:ARG:HE	1:A:79:ARG:HA	1.77	0.40
3:C:252:PHE:CE2	3:C:258:LEU:HD21	2.57	0.40
4:D:145:HIS:O	4:D:147:ARG:N	2.55	0.40
5:E:95:MET:HE3	5:E:95:MET:HA	2.04	0.40
4:D:277:LEU:HG	6:F:134:PHE:CE1	2.57	0.40
7:G:9:ALA:O	7:G:11:PHE:N	2.54	0.40
7:G:60:LYS:O	7:G:61:ASN:C	2.59	0.40
1:A:329:ARG:O	1:A:330:ASP:HB2	2.22	0.40
2:B:286:ILE:HD12	2:B:298:TYR:CE2	2.57	0.40
3:C:185:TRP:CZ3	3:C:235:MET:HG2	2.56	0.40
4:D:65:LYS:CA	4:D:65:LYS:HE2	2.41	0.40
5:E:21:LEU:HD12	5:E:132:TYR:CZ	2.56	0.40
6:F:36:PRO:HG2	6:F:39:GLU:HB2	2.03	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	376/418 (90%)	345 (92%)	29 (8%)	2 (0%)	29	61
2	B	176/394 (45%)	149 (85%)	22 (12%)	5 (3%)	5	19
3	C	337/372 (91%)	306 (91%)	24 (7%)	7 (2%)	7	26
4	D	269/300 (90%)	251 (93%)	17 (6%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	172/178 (97%)	147 (86%)	23 (13%)	2 (1%)	13	40
6	F	163/168 (97%)	150 (92%)	9 (6%)	4 (2%)	5	21
7	G	122/151 (81%)	101 (83%)	14 (12%)	7 (6%)	1	5
All	All	1615/1981 (82%)	1449 (90%)	138 (8%)	28 (2%)	9	31

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	331	LYS
2	B	336	LYS
3	C	65	ASN
6	F	102	PHE
7	G	10	ARG
7	G	22	ASN
2	B	278	VAL
3	C	371	ILE
5	E	87	SER
6	F	32	ARG
6	F	127	TYR
7	G	51	MET
7	G	88	ALA
2	B	335	GLU
3	C	50	GLU
3	C	284	ARG
4	D	146	TYR
6	F	41	ARG
7	G	11	PHE
7	G	63	PRO
1	A	194	PRO
3	C	64	SER
7	G	47	ARG
3	C	179	ARG
2	B	338	SER
3	C	176	VAL
5	E	151	PRO
1	A	216	PRO

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/363 (91%)	307 (93%)	23 (7%)	15	41
2	B	157/345 (46%)	148 (94%)	9 (6%)	20	51
3	C	290/313 (93%)	276 (95%)	14 (5%)	25	58
4	D	241/264 (91%)	235 (98%)	6 (2%)	47	78
5	E	153/159 (96%)	144 (94%)	9 (6%)	19	49
6	F	153/155 (99%)	147 (96%)	6 (4%)	32	66
7	G	106/124 (86%)	96 (91%)	10 (9%)	8	26
All	All	1430/1723 (83%)	1353 (95%)	77 (5%)	22	54

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	LYS
1	A	19	LEU
1	A	25	THR
1	A	68	GLU
1	A	71	THR
1	A	82	ILE
1	A	88	LEU
1	A	117	LEU
1	A	143	VAL
1	A	154	THR
1	A	191	LYS
1	A	230	ARG
1	A	239	VAL
1	A	255	GLN
1	A	282	PHE
1	A	289	ASN
1	A	310	ASP
1	A	318	ASN
1	A	335	LEU
1	A	343	VAL
1	A	363	ILE
1	A	366	GLN
2	B	167	CYS

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Mol	Chain	Res	Type
2	B	182	LEU
2	B	184	ILE
2	B	200	ARG
2	B	220	LEU
2	B	274	GLU
2	B	290	ASP
2	B	320	GLU
2	B	340	PHE
3	C	13	CYS
3	C	21	THR
3	C	30	HIS
3	C	90	LEU
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	175	GLU
3	C	179	ARG
3	C	183	THR
3	C	224	SER
3	C	280	SER
3	C	284	ARG
3	C	367	LYS
4	D	33	VAL
4	D	35	PHE
4	D	49	ASN
4	D	116	LEU
4	D	245	HIS
4	D	265	ARG
5	E	22	LEU
5	E	25	ARG
5	E	82	LEU
5	E	94	GLU
5	E	95	MET
5	E	142	LEU
5	E	144	LEU
5	E	146	GLU
5	E	151	PRO
6	F	6	ARG
6	F	101	PHE
6	F	102	PHE
6	F	125	GLN
6	F	147	SER

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Mol	Chain	Res	Type
6	F	152	SER
7	G	18	GLU
7	G	21	GLU
7	G	45	CYS
7	G	46	LEU
7	G	64	ILE
7	G	68	SER
7	G	86	PHE
7	G	87	LYS
7	G	90	ASP
7	G	122	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	144	GLN
1	A	205	GLN
1	A	206	GLN
1	A	243	ASN
1	A	255	GLN
1	A	289	ASN
1	A	306	ASN
1	A	318	ASN
1	A	370	HIS
2	B	165	HIS
2	B	205	ASN
2	B	231	GLN
2	B	284	ASN
2	B	323	GLN
3	C	44	GLN
3	C	46	HIS
3	C	65	ASN
3	C	107	ASN
3	C	222	HIS
3	C	331	GLN
4	D	140	ASN
4	D	202	HIS
4	D	231	HIS
4	D	242	ASN
5	E	138	GLN
5	E	167	GLN

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Mol	Chain	Res	Type
6	F	28	GLN
6	F	78	GLN
6	F	125	GLN
6	F	129	HIS
7	G	22	ASN
7	G	48	GLN
7	G	56	GLN
7	G	65	ASN
7	G	96	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	8	24,29,29	1.31	2 (8%)	29,45,45	1.60	5 (17%)
9	ADP	B	395	-	24,29,29	1.38	3 (12%)	29,45,45	1.50	4 (13%)

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	8	-	0/12/32/32	0/3/3/3
9	ADP	B	395	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	395	ADP	C2-N1	3.69	1.40	1.33
9	A	501	ADP	C2-N1	3.47	1.40	1.33
9	B	395	ADP	PB-O1B	3.30	1.61	1.50
9	A	501	ADP	PB-O1B	3.18	1.60	1.50
9	B	395	ADP	O4'-C1'	2.40	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	395	ADP	N3-C2-N1	-5.47	120.13	128.68
9	A	501	ADP	N3-C2-N1	-5.40	120.24	128.68
9	A	501	ADP	O4'-C1'-C2'	-3.20	102.24	106.93
9	A	501	ADP	PA-O3A-PB	-3.09	122.22	132.83
9	B	395	ADP	PA-O3A-PB	-2.89	122.92	132.83
9	A	501	ADP	O3B-PB-O3A	2.84	114.15	104.64
9	B	395	ADP	O3B-PB-O3A	2.22	112.06	104.64
9	B	395	ADP	C4-C5-N7	-2.19	107.12	109.40
9	A	501	ADP	C3'-C2'-C1'	-2.08	97.85	100.98

There are no chirality outliers.

There are no torsion outliers.

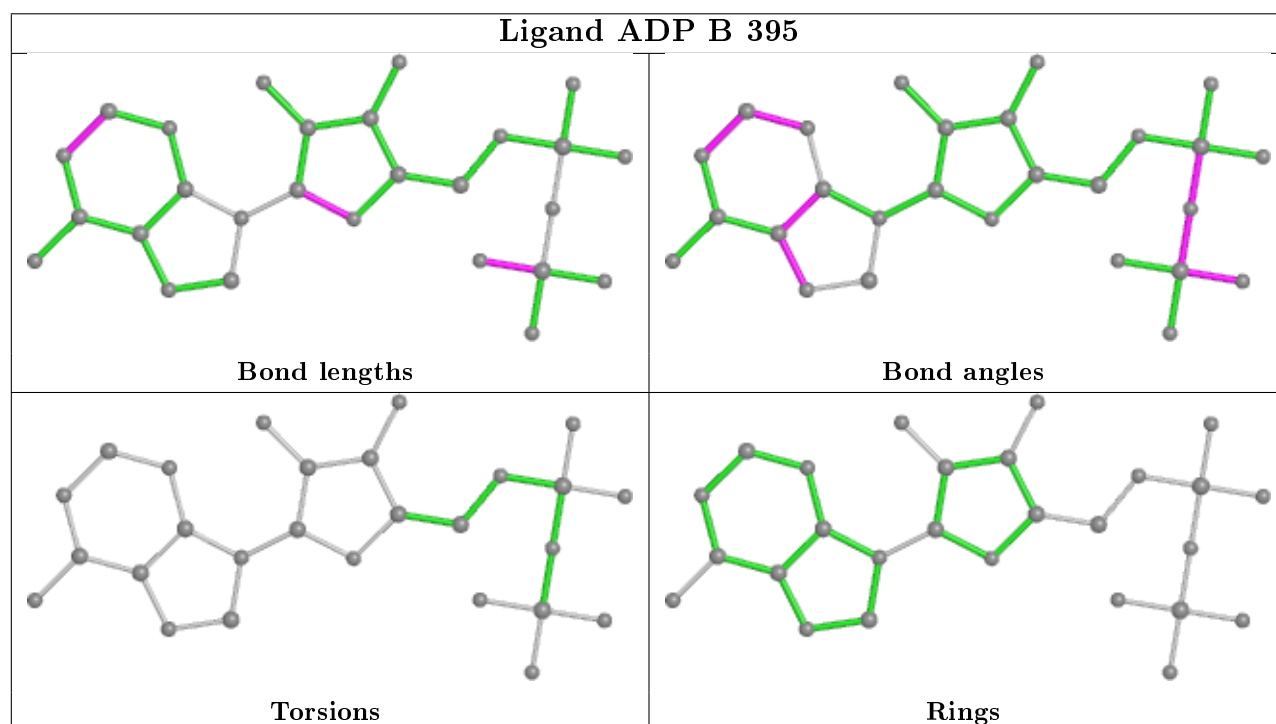
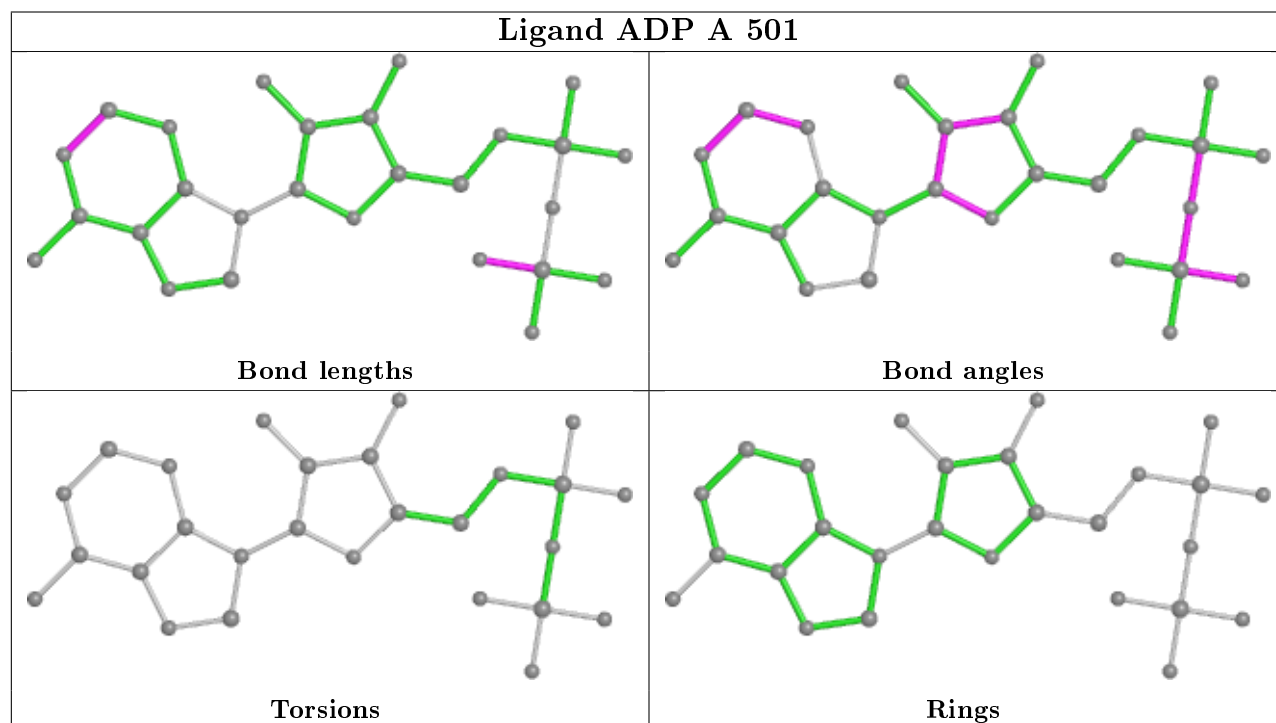
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	501	ADP	3	0
9	B	395	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/418 (92%)	-0.02	4 (1%) 82 82	30, 56, 84, 103	0
2	B	184/394 (46%)	0.43	26 (14%) 2 2	34, 64, 113, 121	0
3	C	341/372 (91%)	-0.06	3 (0%) 84 84	30, 47, 80, 103	0
4	D	273/300 (91%)	-0.09	1 (0%) 92 93	33, 53, 81, 95	0
5	E	174/178 (97%)	0.31	9 (5%) 27 23	42, 70, 96, 105	0
6	F	165/168 (98%)	-0.13	0 100 100	37, 52, 68, 79	0
7	G	128/151 (84%)	0.45	12 (9%) 8 6	42, 80, 106, 118	0
All	All	1653/1981 (83%)	0.07	55 (3%) 46 41	30, 56, 94, 121	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	10	ARG	5.0
2	B	337	LEU	3.8
2	B	278	VAL	3.7
2	B	176	PRO	3.7
5	E	175	GLY	3.6
2	B	343	ARG	3.5
5	E	85	CYS	3.4
5	E	96	TYR	3.4
5	E	86	ASN	3.2
1	A	52	MET	3.2
1	A	39	GLU	3.1
2	B	290	ASP	3.1
7	G	13	LYS	3.0
2	B	328	ARG	2.9
3	C	127	GLN	2.9
3	C	372	VAL	2.9
2	B	165	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	340	PHE	2.8
5	E	154	ASP	2.8
2	B	329	VAL	2.8
2	B	166	ILE	2.7
7	G	49	GLY	2.7
2	B	281	LEU	2.7
2	B	155	VAL	2.6
2	B	276	VAL	2.6
1	A	70	PRO	2.6
2	B	285	THR	2.5
4	D	283	ASP	2.5
7	G	9	ALA	2.5
7	G	11	PHE	2.5
7	G	149	LYS	2.4
2	B	339	LYS	2.4
2	B	184	ILE	2.4
5	E	82	LEU	2.4
2	B	288	ALA	2.3
5	E	93	LYS	2.3
7	G	46	LEU	2.2
7	G	151	VAL	2.2
7	G	22	ASN	2.2
2	B	182	LEU	2.2
2	B	302	VAL	2.2
1	A	80	HIS	2.1
2	B	181	ARG	2.1
2	B	277	GLY	2.1
5	E	25	ARG	2.1
2	B	174	SER	2.1
7	G	43	ASP	2.1
7	G	66	THR	2.1
2	B	336	LYS	2.1
5	E	84	LYS	2.1
3	C	362	LEU	2.1
7	G	47	ARG	2.1
2	B	324	LEU	2.1
2	B	286	ILE	2.0
2	B	169	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

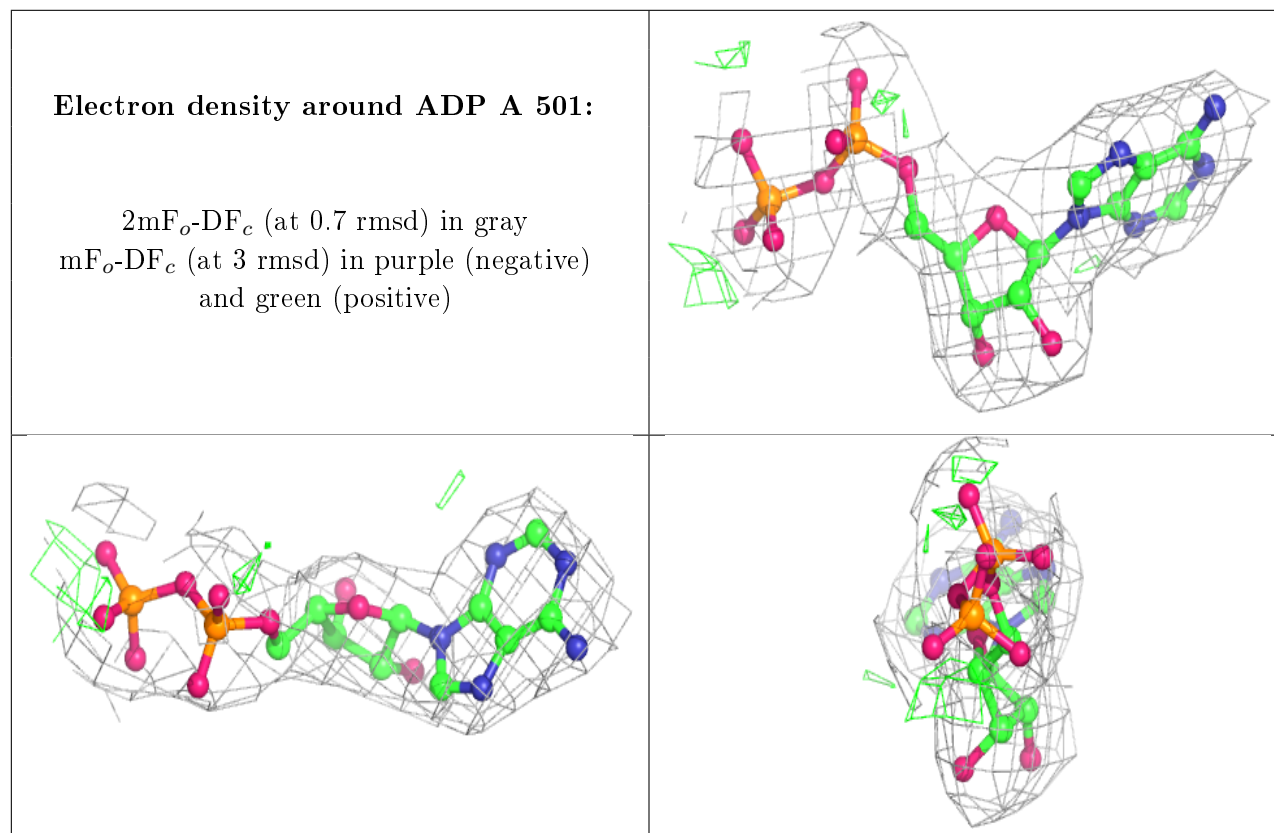
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

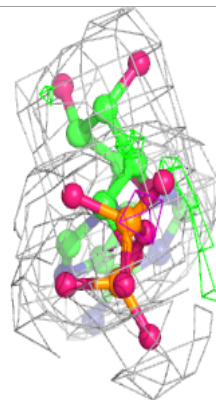
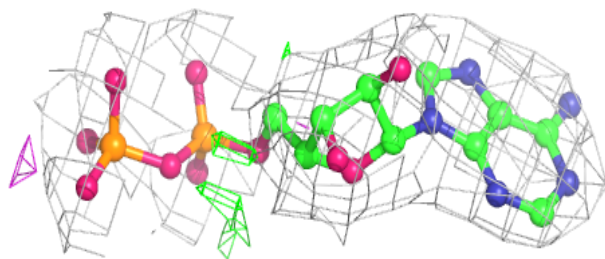
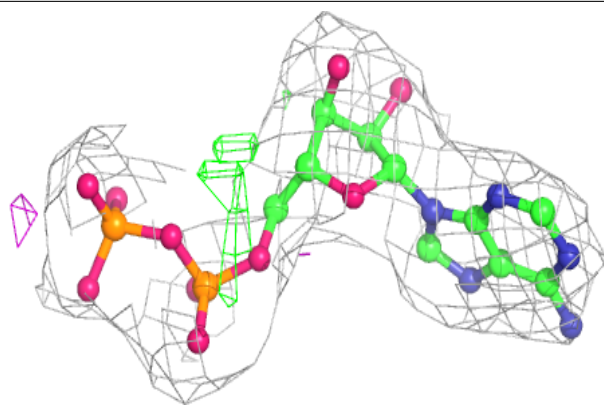
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	ADP	A	501	27/27	0.92	0.20	50,56,68,70	0
9	ADP	B	395	27/27	0.94	0.12	59,64,77,78	0
8	CA	A	500	1/1	0.97	0.38	73,73,73,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around ADP B 395:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.