



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:37 AM UTC

PDB ID : 2P9N / pdb_00002p9n
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

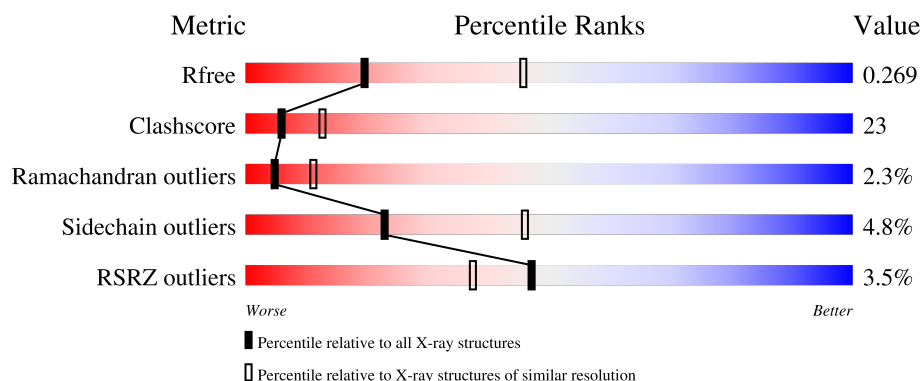
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	4% 54% 36% 5% 5%
2	B	394	5% 27% 19% 5% 48%
3	C	372	% 51% 37% • 8%
4	D	300	% 58% 34% • 6%
5	E	178	3% 50% 42% • • •

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Mol	Chain	Length	Quality of chain
6	F	168	% 69% 27%
7	G	151	7% 56% 25% 7% 11%

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			

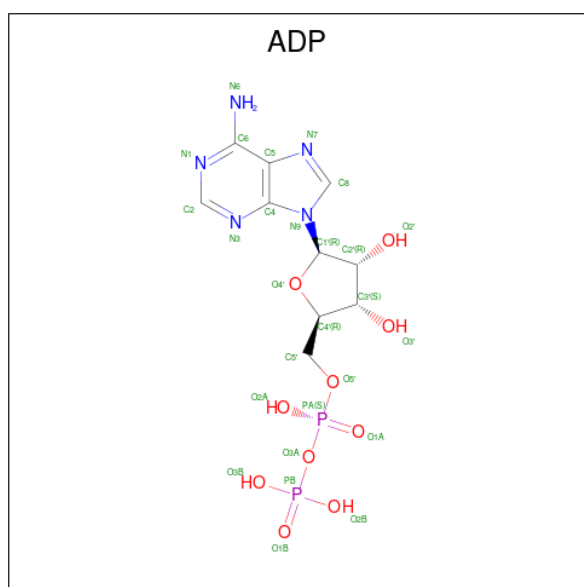
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

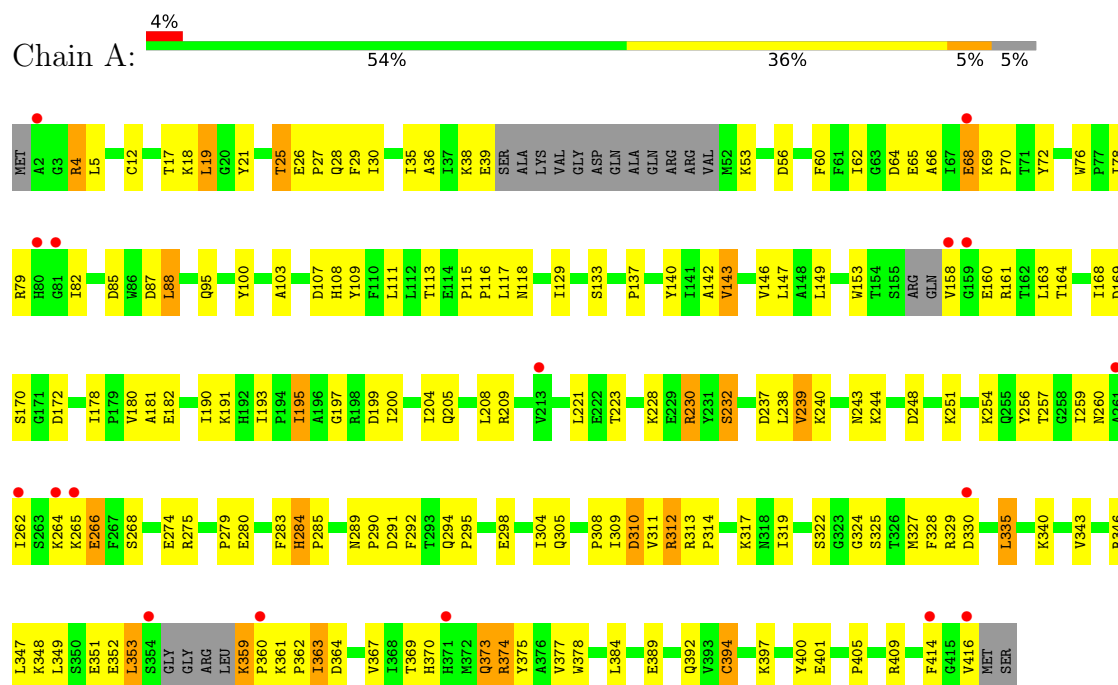


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

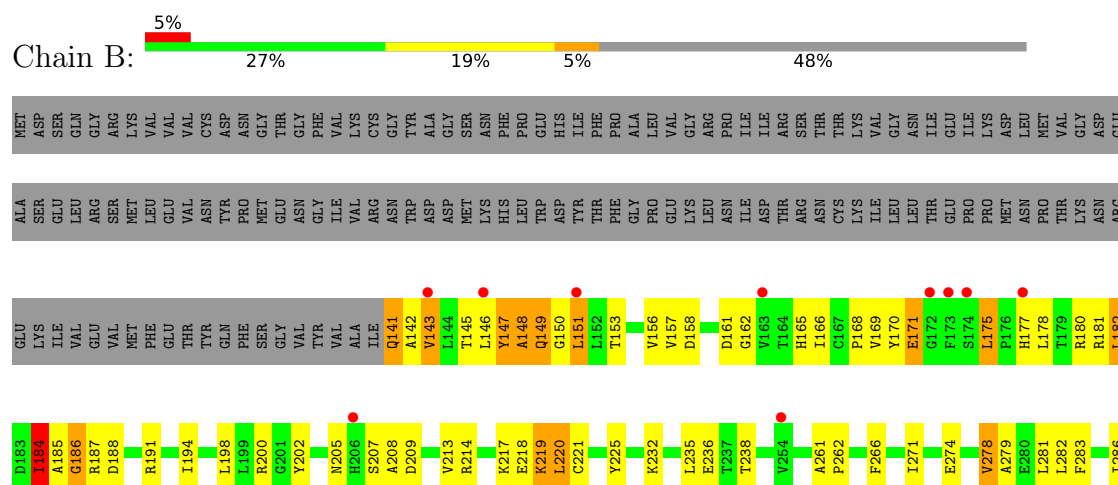
3 Residue-property plots [i](#)

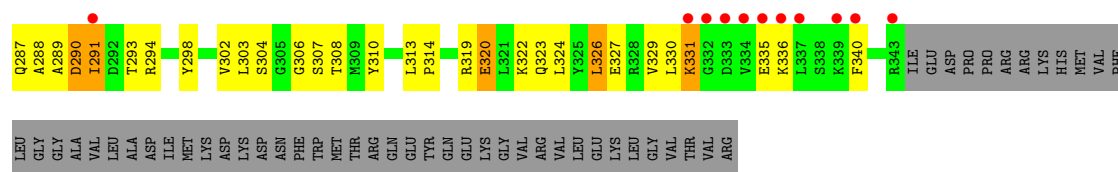
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

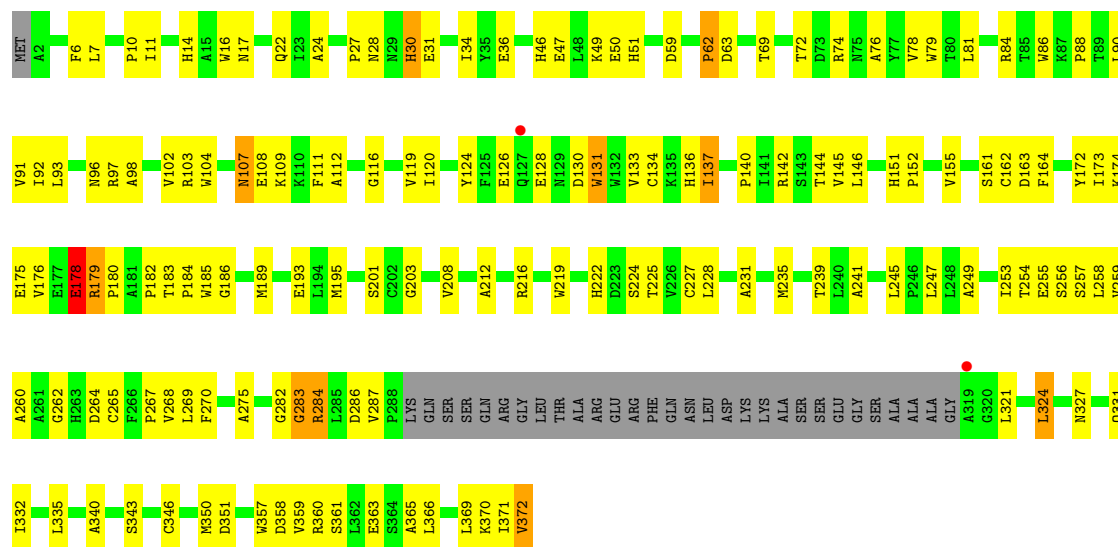


• Molecule 2: Actin-like protein 2

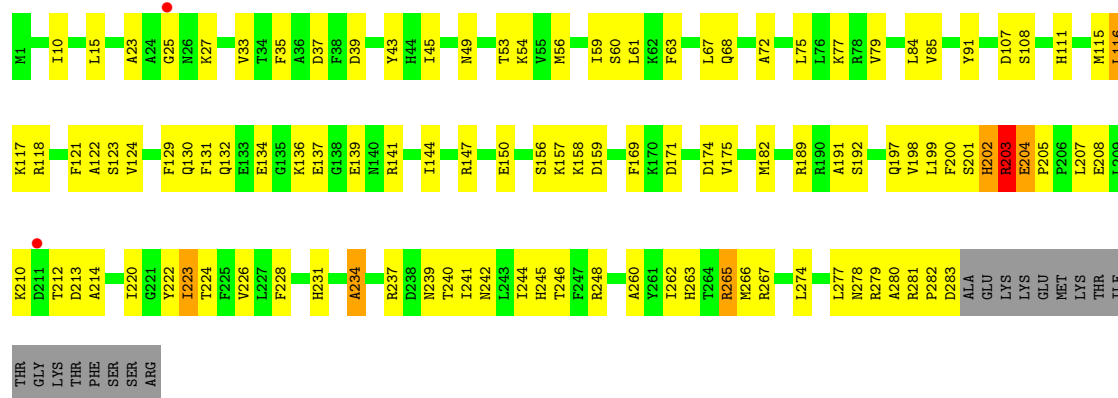




• Molecule 3: Actin-related protein 2/3 complex subunit 1B

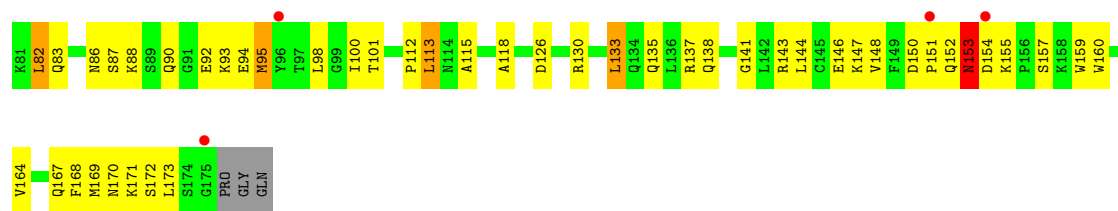


• Molecule 4: Actin-related protein 2/3 complex subunit 2



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

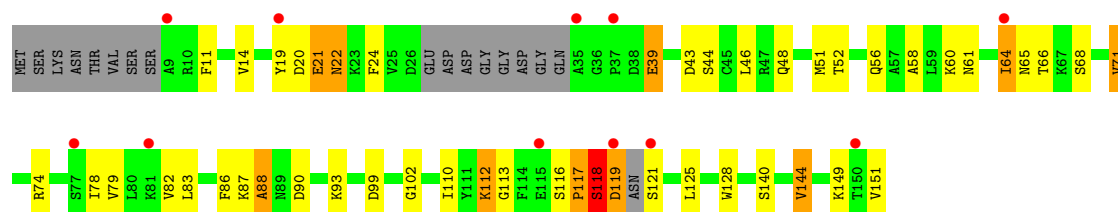




• Molecule 6: Actin-related protein 2/3 complex subunit 4



• 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, α , β , γ	111.13Å 129.27Å 203.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.85) 93.1 (50.00-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	3465 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ADP, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	0/3257	0.96	9/4418 (0.2%)
2	B	0.43	0/1600	0.97	5/2167 (0.2%)
3	C	0.46	0/2717	1.03	12/3688 (0.3%)
4	D	0.49	0/2336	0.98	11/3154 (0.3%)
5	E	0.41	0/1441	0.91	7/1941 (0.4%)
6	F	0.53	0/1393	1.01	10/1868 (0.5%)
7	G	0.63	4/1034 (0.4%)	1.07	5/1389 (0.4%)
All	All	0.48	4/13778 (0.0%)	0.99	59/18625 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	118	SER	C-O	-8.88	1.12	1.24
7	G	118	SER	N-CA	-7.13	1.36	1.46
7	G	119	ASP	N-CA	6.21	1.54	1.46
7	G	117	PRO	CA-C	-5.67	1.45	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	204	GLU	N-CA-C	-12.88	90.94	109.62
7	G	116	SER	CA-C-N	-12.39	107.77	120.03
7	G	116	SER	C-N-CA	-12.39	107.77	120.03
2	B	149	GLN	N-CA-C	-11.43	99.31	113.02
6	F	101	PHE	N-CA-C	-8.74	96.42	110.32
4	D	279	ARG	N-CA-C	-8.44	102.98	113.20
3	C	283	GLY	N-CA-C	7.58	126.36	112.27
3	C	137	ILE	N-CA-C	-7.25	96.64	107.37
6	F	44	LYS	N-CA-C	7.17	121.67	112.34
3	C	30	HIS	N-CA-C	-7.10	104.36	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	GLU	N-CA-C	-7.01	103.72	111.36
1	A	118	ASN	N-CA-C	-6.94	99.23	110.20
4	D	129	PHE	N-CA-C	-6.94	103.80	111.36
2	B	151	LEU	N-CA-C	-6.91	98.14	108.99
3	C	11	ILE	N-CA-C	-6.88	97.26	107.51
5	E	63	GLU	N-CA-C	-6.75	104.52	112.89
3	C	287	VAL	N-CA-C	6.72	114.41	108.63
7	G	118	SER	CA-C-O	-6.65	111.00	120.51
6	F	131	LEU	N-CA-C	-6.39	104.39	111.36
5	E	22	LEU	CA-C-N	6.31	126.67	119.92
5	E	22	LEU	C-N-CA	6.31	126.67	119.92
6	F	101	PHE	CA-C-N	-6.10	112.66	122.24
6	F	101	PHE	C-N-CA	-6.10	112.66	122.24
3	C	130	ASP	N-CA-C	6.04	119.57	111.24
2	B	209	ASP	N-CA-C	6.01	119.57	112.72
1	A	284	HIS	CA-C-N	6.01	127.35	119.84
1	A	284	HIS	C-N-CA	6.01	127.35	119.84
6	F	102	PHE	N-CA-C	-5.96	106.62	114.31
1	A	76	TRP	CA-C-N	5.96	126.11	119.32
1	A	76	TRP	C-N-CA	5.96	126.11	119.32
6	F	79	ALA	N-CA-C	5.90	117.79	111.36
1	A	312	ARG	N-CA-C	5.89	118.18	111.11
2	B	219	LYS	N-CA-C	5.85	118.89	111.69
3	C	245	LEU	CA-C-N	5.79	125.72	119.76
3	C	245	LEU	C-N-CA	5.79	125.72	119.76
4	D	203	ARG	N-CA-C	5.78	123.10	110.80
6	F	109	VAL	N-CA-C	-5.77	102.08	109.30
5	E	173	LEU	N-CA-C	-5.77	106.20	113.18
4	D	33	VAL	N-CA-C	5.73	116.93	108.45
3	C	178	GLU	N-CA-C	5.72	117.67	109.14
4	D	79	VAL	N-CA-C	5.68	115.87	110.42
3	C	78	VAL	N-CA-C	-5.67	100.41	108.58
4	D	122	ALA	N-CA-C	5.67	117.92	111.11
5	E	160	TRP	N-CA-C	-5.65	105.67	113.18
3	C	163	ASP	N-CA-C	-5.58	105.78	112.59
2	B	142	ALA	N-CA-C	-5.58	105.35	111.82
7	G	112	LYS	N-CA-C	-5.44	105.35	111.28
4	D	107	ASP	N-CA-C	5.42	117.18	111.28
7	G	144	VAL	N-CA-C	-5.34	105.18	111.00
6	F	167	ASN	N-CA-C	5.32	119.61	113.18
5	E	16	ILE	N-CA-C	-5.28	98.32	106.72
1	A	232	SER	N-CA-C	5.28	117.10	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	27	LYS	CA-C-N	5.25	125.55	119.93
4	D	27	LYS	C-N-CA	5.25	125.55	119.93
4	D	39	ASP	N-CA-C	5.21	118.31	111.28
6	F	42	SER	N-CA-C	5.21	118.76	112.93
3	C	253	ILE	N-CA-C	-5.16	108.10	113.10
1	A	373	GLN	N-CA-C	5.14	117.62	111.71
5	E	19	MET	N-CA-C	-5.06	102.28	110.32

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	155	0
2	B	1572	0	1559	95	0
3	C	2648	0	2602	141	0
4	D	2287	0	2252	80	0
5	E	1408	0	1408	80	0
6	F	1371	0	1410	42	0
7	G	1023	0	1041	48	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	617	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 (617) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:107:ASN:C	3:C:107:ASN:HD22	1.87	0.82
3:C:185:TRP:HE3	3:C:235:MET:HE2	1.44	0.82
1:A:4:ARG:HH11	1:A:4:ARG:HB2	1.44	0.82
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:HD13	1:A:363:ILE:H	1.46	0.79
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.65	0.78
2:B:161:ASP:OD2	9:B:395:ADP:H3'	1.84	0.78
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.65	0.78
4:D:228:PHE:H	4:D:231:HIS:HD2	1.31	0.78
5:E:150:ASP:C	5:E:152:GLN:H	1.89	0.78
1:A:257:THR:HG22	1:A:268:SER:HB3	1.66	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
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.67	0.77
3:C:96:ASN:O	3:C:97:ARG:HD3	1.85	0.77
3:C:14:HIS:H	3:C:331:GLN:NE2	1.82	0.77
5:E:152:GLN:HB3	5:E:155:LYS:HZ3	1.49	0.76
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
4:D:281:ARG:C	4:D:283:ASP:H	1.93	0.75
1:A:384:LEU:HB3	1:A:414:PHE:CZ	2.22	0.74
1:A:343:VAL:CG2	1:A:363:ILE:HG13	2.17	0.74
3:C:371:ILE:O	3:C:372:VAL:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:116:PRO:O	1:A:117:LEU:HB2	1.87	0.73
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.18	0.73
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.70	0.73
7:G:46:LEU:HD23	7:G:51:MET:HE1	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
1:A:313:ARG:HH12	1:A:363:ILE:HA	1.55	0.72
3:C:269:LEU:H	3:C:283:GLY:CA	2.03	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:H	1:A:363:ILE:CD1	2.03	0.71
1:A:223:THR:HG23	1:A:256:TYR:HE2	1.54	0.71
3:C:144:THR:H	6:F:28:GLN:NE2	1.89	0.71
3:C:119:VAL:HG21	3:C:136:HIS:HB3	1.72	0.71
6:F:101:PHE:HB3	6:F:104:LEU:HB2	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
2:B:147:TYR:C	2:B:149:GLN:H	2.00	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
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.26	0.69
1:A:87:ASP:OD2	4:D:267:ARG:HD2	1.93	0.69
1:A:230:ARG:HH11	1:A:230:ARG:HB3	1.57	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:126:GLU:HB2	3:C:131:TRP:CZ3	2.29	0.67
3:C:144:THR:H	6:F:28:GLN:HE22	1.42	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:HH11	1:A:230:ARG:CB	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HH11	1:A:4:ARG:CB	2.07	0.67
3:C:14:HIS:N	3:C:331:GLN:HE22	1.89	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
2:B:326:LEU:HD23	2:B:326:LEU:C	2.21	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
2:B:291:ILE:HD12	2:B:294:ARG:HH11	1.60	0.65
7:G:87:LYS:HD3	7:G:87:LYS:N	2.11	0.65
1:A:30:ILE:HD13	1:A:375:TYR:CZ	2.31	0.65
1:A:78:ILE:O	1:A:79:ARG:HD2	1.97	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
1:A:363:ILE:HD13	1:A:363:ILE:N	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
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:153:ASN:O	5:E:155:LYS:HG3	1.96	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
5:E:150:ASP:O	5:E:152:GLN:N	2.29	0.65
1:A:359:LYS:NZ	1:A:359:LYS:HB3	2.12	0.65
3:C:185:TRP:CE3	3:C:235:MET:HE2	2.28	0.64
3:C:131:TRP:HE3	3:C:131:TRP:O	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:151:HIS:CE1	3:C:152:PRO:HG2	2.33	0.64
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.79	0.64
4:D:68:GLN:HA	4:D:72:ALA:HB3	1.79	0.64
5:E:95:MET:HE3	5:E:95:MET:HA	1.80	0.64
6:F:20:LEU:HD12	6:F:132:VAL:HG22	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:165:HIS:CD2	2:B:181:ARG:HG2	2.34	0.62
4:D:198:VAL:C	4:D:199:LEU:HD12	2.24	0.62
1:A:82:ILE:HD12	1:A:115:PRO:HG3	1.80	0.62
3:C:201:SER:HB3	7:G:149:LYS:HZ3	1.62	0.62
3:C:268:VAL:HA	3:C:284:ARG:H	1.65	0.62
4:D:282:PRO:O	4:D:283:ASP:HB2	1.99	0.62
1:A:348:LYS:HG2	1:A:352:GLU:OE2	2.00	0.61
4:D:132:GLN:NE2	4:D:159:ASP:HA	2.14	0.61
2:B:161:ASP:HA	2:B:186:GLY:HA3	1.81	0.61
6:F:96:MET:HG2	6:F:96:MET:O	1.99	0.61
5:E:150:ASP:C	5:E:152:GLN:N	2.58	0.61
1:A:27:PRO:HG3	1:A:378:TRP:CD2	2.35	0.61
4:D:53:THR:C	4:D:54:LYS:HD2	2.26	0.60
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.83	0.60
6:F:2:THR:C	6:F:4:THR:H	2.08	0.60
1:A:289:ASN:HD22	1:A:289:ASN:C	2.08	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:47:GLU:OE2	3:C:49:LYS:HE3	2.02	0.60
3:C:107:ASN:HD22	3:C:109:LYS:H	1.49	0.60
4:D:111:HIS:CD2	4:D:115:MET:HE2	2.37	0.60
5:E:24:ILE:CG2	5:E:32:ALA:HB1	2.32	0.59
1:A:374:ARG:CG	1:A:374:ARG:HH11	2.15	0.59
5:E:146:GLU:HG3	5:E:147:LYS:N	2.17	0.59
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.37	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
6:F:60:LYS:HE3	6:F:112:TYR:CE2	2.36	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
5:E:167:GLN:NE2	5:E:172:SER:HB2	2.18	0.58
6:F:125:GLN:HE21	6:F:125:GLN:HA	1.67	0.58
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.68	0.58
3:C:254:THR:OG1	3:C:372:VAL:HG13	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:228:LYS:O	1:A:232:SER:HB2	2.04	0.57
2:B:175:LEU:HB2	2:B:177:HIS:CE1	2.39	0.57
3:C:178:GLU:O	3:C:179:ARG:C	2.47	0.57
1:A:309:ILE:HB	1:A:312:ARG:HH21	1.69	0.57
3:C:186:GLY:O	3:C:189:MET:HE2	2.05	0.57
1:A:28:GLN:HG2	4:D:10:ILE:HD13	1.85	0.57
1:A:374:ARG:HG3	1:A:374:ARG:NH1	2.19	0.57
3:C:282:GLY:HA3	3:C:370:LYS:HZ1	1.69	0.57
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.20	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
1:A:304:ILE:HG22	1:A:312:ARG:HG2	1.86	0.56
3:C:284:ARG:NH1	3:C:286:ASP:O	2.37	0.56
3:C:107:ASN:ND2	3:C:107:ASN:C	2.57	0.56
3:C:107:ASN:HD22	3:C:108:GLU:N	2.02	0.56
4:D:248:ARG:HD3	4:D:248:ARG:C	2.29	0.56
1:A:205:GLN:NE2	1:A:221:LEU:HG	2.21	0.56
3:C:193:GLU:HB3	3:C:195:MET:HE2	1.88	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
3:C:228:LEU:C	3:C:228:LEU:HD23	2.31	0.56
1:A:305:GLN:HA	1:A:312:ARG:HD3	1.87	0.56
3:C:59:ASP:OD2	3:C:104:TRP:N	2.32	0.56
3:C:84:ARG:O	3:C:84:ARG:HG2	2.06	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
2:B:158:ASP:HA	2:B:304:SER:O	2.06	0.55
4:D:281:ARG:C	4:D:283:ASP:N	2.63	0.55
5:E:112:PRO:O	5:E:113:LEU:CB	2.55	0.55
4:D:156:SER:C	4:D:157:LYS:HD2	2.31	0.55
6:F:101:PHE:CB	6:F:104:LEU:HB2	2.35	0.55
3:C:371:ILE:C	3:C:372:VAL:CG2	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:191:ARG:O	2:B:194:ILE:HB	2.08	0.53
3:C:92:ILE:H	3:C:92:ILE:CD1	2.17	0.53
4:D:67:LEU:HD23	4:D:144:ILE:HD12	1.88	0.53
5:E:16:ILE:HG23	5:E:16:ILE:O	2.07	0.53
1:A:18:LYS:N	1:A:18:LYS:HD3	2.24	0.53
7:G:87:LYS:N	7:G:87:LYS:CD	2.71	0.53
4:D:45:ILE:HA	4:D:56:MET:O	2.07	0.53
3:C:175:GLU:OE1	3:C:175:GLU:N	2.42	0.53
3:C:371:ILE:N	3:C:371:ILE:HD12	2.24	0.53
1:A:262:ILE:C	1:A:264:LYS:H	2.16	0.53
6:F:53:ILE:N	6:F:53:ILE:HD12	2.23	0.53
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.44	0.53
1:A:248:ASP:OD1	1:A:251:LYS:HD3	2.09	0.53
6:F:145:GLU:HG3	6:F:149:MET:HE2	1.90	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
4:D:203:ARG:C	4:D:203:ARG:HD3	2.34	0.53
5:E:25:ARG:NH1	5:E:38:ASP:HA	2.18	0.53
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
4:D:37:ASP:HB2	4:D:43:TYR:HE1	1.73	0.52
5:E:18:ASN:O	5:E:63:GLU:HB3	2.09	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
7:G:68:SER:CB	7:G:71:VAL:HG12	2.39	0.52
1:A:329:ARG:O	1:A:330:ASP:HB2	2.10	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
6:F:146:ILE:HA	6:F:149:MET:HE3	1.91	0.52
2:B:175:LEU:HD23	2:B:175:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:239:VAL:HG23	1:A:240:LYS:H	1.75	0.51
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.92	0.51
7:G:87:LYS:O	7:G:88:ALA:C	2.54	0.51
2:B:278:VAL:HG13	2:B:279:ALA:N	2.25	0.51
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.75	0.51
1:A:36:ALA:HB2	1:A:66:ALA:HB1	1.93	0.51
2:B:279:ALA:CB	2:B:320:GLU:HG2	2.41	0.51
1:A:62:ILE:HD11	1:A:100:TYR:CE2	2.45	0.51
1:A:208:LEU:HD21	1:A:274:GLU:OE2	2.11	0.51
1:A:140:TYR:HB2	1:A:394:CYS:SG	2.51	0.50
1:A:289:ASN:ND2	1:A:291:ASP:H	2.09	0.50
1:A:289:ASN:C	1:A:289:ASN:ND2	2.69	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
1:A:164:THR:HG23	1:A:181:ALA:HA	1.93	0.50
2:B:184:ILE:HD13	2:B:271:ILE:HD13	1.92	0.50
4:D:118:ARG:HD3	4:D:118:ARG:C	2.37	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
7:G:78:ILE:O	7:G:82:VAL:HG23	2.11	0.50
1:A:359:LYS:HB3	1:A:359:LYS:HZ3	1.77	0.50
1:A:374:ARG:CG	1:A:374:ARG:NH1	2.74	0.50
4:D:201:SER:O	4:D:202:HIS:C	2.55	0.50
5:E:144:LEU:O	5:E:148:VAL:HG23	2.11	0.50
7:G:11:PHE:O	7:G:14:VAL:HG12	2.12	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:HG22	3:C:120:ILE:N	2.27	0.50
3:C:257:SER:OG	3:C:372:VAL:N	2.44	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:119:VAL:CG2	3:C:136:HIS:HB3	2.40	0.50
1:A:397:LYS:O	1:A:401:GLU:HG3	2.12	0.50
3:C:92:ILE:HD12	3:C:92:ILE:N	2.19	0.50
3:C:258:LEU:HB2	3:C:270:PHE:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:52:THR:HG22	7:G:52:THR:O	2.12	0.50
7:G:119:ASP:C	7:G:121:SER:N	2.70	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
3:C:72:THR:HA	3:C:98:ALA:HB1	1.93	0.49
3:C:343:SER:O	3:C:359:VAL:HG23	2.12	0.49
7:G:44:SER:O	7:G:48:GLN:HG3	2.13	0.49
5:E:35:GLU:HG3	5:E:37:LYS:O	2.12	0.49
4:D:212:THR:C	4:D:214:ALA:H	2.20	0.49
7:G:118:SER:O	7:G:119:ASP:CG	2.56	0.49
1:A:309:ILE:HG23	1:A:310:ASP:H	1.77	0.49
3:C:14:HIS:HA	3:C:24:ALA:O	2.12	0.49
3:C:34:ILE:HB	3:C:46:HIS:HB2	1.95	0.49
3:C:282:GLY:HA3	3:C:370:LYS:HZ3	1.75	0.49
4:D:208:GLU:OE2	4:D:208:GLU:N	2.38	0.49
7:G:46:LEU:HD23	7:G:51:MET:CE	2.39	0.49
4:D:189:ARG:C	4:D:191:ALA:H	2.19	0.49
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.95	0.49
2:B:161:ASP:OD2	9:B:395:ADP:C3'	2.57	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:82:LEU:HB3	5:E:148:VAL:HG11	1.94	0.49
5:E:152:GLN:HB3	5:E:155:LYS:CE	2.43	0.49
4:D:203:ARG:C	4:D:203:ARG:CD	2.86	0.48
1:A:12:CYS:HB3	1:A:78:ILE:CD1	2.43	0.48
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.48	0.48
5:E:95:MET:HG3	5:E:141:GLY:HA3	1.95	0.48
6:F:20:LEU:HD12	6:F:132:VAL:CG2	2.42	0.48
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.48	0.48
1:A:343:VAL:O	1:A:347:LEU:HD13	2.13	0.48
1:A:108:HIS:O	1:A:137:PRO:HD2	2.13	0.48
1:A:327:MET:HE3	1:A:327:MET:HA	1.95	0.48
2:B:310:TYR:CE1	9:B:395:ADP:H2	2.31	0.48
3:C:358:ASP:HB3	3:C:361:SER:CB	2.44	0.48
4:D:240:THR:O	4:D:244:ILE:HG22	2.13	0.48
1:A:308:PRO:HG2	2:B:207:SER:HB2	1.95	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
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:HA	1:A:79:ARG:NE	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:GLN:O	5:E:93:LYS:HB2	2.13	0.48
7:G:74:ARG:O	7:G:78:ILE:HG13	2.13	0.48
2:B:147:TYR:C	2:B:149:GLN:N	2.68	0.47
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:18:ASN:CG	5:E:118:ALA:H	2.21	0.47
1:A:107:ASP:CG	4:D:147:ARG:HH22	2.22	0.47
1:A:370:HIS:O	1:A:373:GLN:HG3	2.14	0.47
4:D:134:GLU:HB2	4:D:136:LYS:HG3	1.96	0.47
5:E:24:ILE:HG23	5:E:32:ALA:HB1	1.97	0.47
1:A:190:ILE:HG22	1:A:191:LYS:N	2.29	0.47
5:E:30:GLY:C	5:E:32:ALA:H	2.22	0.47
7:G:71:VAL:O	7:G:74:ARG:HB3	2.14	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
3:C:254:THR:HG1	3:C:257:SER:H	1.61	0.47
7:G:86:PHE:C	7:G:87:LYS:HD3	2.39	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
2:B:170:TYR:O	2:B:171:GLU:C	2.58	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
3:C:133:VAL:O	3:C:134:CYS:HB3	2.15	0.47
3:C:324:LEU:HD22	3:C:357:TRP:CH2	2.50	0.47
1:A:53:LYS:O	1:A:56:ASP:OD2	2.33	0.46
3:C:10:PRO:HD2	3:C:28:ASN:ND2	2.30	0.46
3:C:222:HIS:C	3:C:224:SER:H	2.23	0.46
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.49	0.46
1:A:111:LEU:HD23	1:A:111:LEU:C	2.39	0.46
2:B:153:THR:HA	2:B:169:VAL:O	2.15	0.46
2:B:286:ILE:O	2:B:289:ALA:HB3	2.15	0.46
5:E:38:ASP:OD2	5:E:38:ASP:N	2.44	0.46
6:F:125:GLN:HA	6:F:125:GLN:NE2	2.31	0.46
6:F:161:ALA:O	6:F:165:LEU:HD22	2.15	0.46
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
1:A:361:LYS:HD3	1:A:361:LYS:C	2.40	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
2:B:266:PHE:HD1	2:B:320:GLU:OE2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:LEU:HD12	2:B:308:THR:CB	2.43	0.46
3:C:371:ILE:O	3:C:372:VAL:CG2	2.62	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
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.46	0.46
3:C:79:TRP:CZ3	3:C:88:PRO:HB3	2.50	0.46
1:A:68:GLU:H	1:A:68:GLU:CD	2.16	0.46
2:B:148:ALA:C	2:B:150:GLY:H	2.23	0.46
3:C:208:VAL:HG12	3:C:219:TRP:HB3	1.96	0.46
1:A:170:SER:OG	1:A:325:SER:HB2	2.16	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
5:E:100:ILE:HD11	5:E:138:GLN:OE1	2.15	0.46
5:E:126:ASP:OD2	5:E:130:ARG:NH1	2.48	0.46
7:G:58:ALA:HB1	7:G:79:VAL:HG22	1.98	0.46
1:A:311:VAL:C	1:A:314:PRO:HD2	2.40	0.45
1:A:35:ILE:HG21	1:A:88:LEU:HG	1.97	0.45
1:A:200:ILE:O	1:A:204:ILE:HG13	2.17	0.45
3:C:6:PHE:O	3:C:7:LEU:HB3	2.15	0.45
3:C:151:HIS:CG	3:C:152:PRO:HD2	2.51	0.45
3:C:172:TYR:C	3:C:172:TYR:CD2	2.94	0.45
3:C:173:ILE:O	3:C:176:VAL:HG22	2.17	0.45
3:C:283:GLY:O	3:C:284:ARG:HB2	2.15	0.45
4:D:202:HIS:O	4:D:203:ARG:CB	2.61	0.45
7:G:66:THR:HG21	7:G:71:VAL:HG21	1.99	0.45
1:A:254:LYS:HG2	1:A:275:ARG:NH1	2.31	0.45
2:B:143:VAL:O	2:B:147:TYR:CB	2.64	0.45
3:C:225:THR:HG22	3:C:241:ALA:HA	1.99	0.45
3:C:247:LEU:HA	3:C:262:GLY:HA3	1.99	0.45
1:A:274:GLU:OE1	1:A:274:GLU:N	2.44	0.45
4:D:202:HIS:C	4:D:202:HIS:ND1	2.74	0.45
7:G:52:THR:O	7:G:56:GLN:HG3	2.17	0.45
7:G:64:ILE:O	7:G:149:LYS:HB3	2.17	0.45
2:B:182:LEU:HD11	2:B:278:VAL:N	2.31	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
3:C:145:VAL:HA	3:C:161:SER:HB3	1.99	0.45
3:C:260:ALA:O	3:C:267:PRO:HA	2.16	0.45
4:D:278:ASN:C	4:D:280:ALA:H	2.24	0.45
7:G:121:SER:O	7:G:125:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:VAL:HB	6:F:33:HIS:HB2	1.99	0.45
1:A:21:TYR:OH	1:A:103:ALA:HB2	2.17	0.45
1:A:285:PRO:HG2	1:A:294:GLN:O	2.16	0.45
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.16	0.45
7:G:39:GLU:HG2	7:G:78:ILE:CD1	2.47	0.45
2:B:146:LEU:O	2:B:151:LEU:O	2.34	0.45
2:B:238:THR:HG22	6:F:106:ARG:NH2	2.32	0.45
4:D:245:HIS:CE1	4:D:246:THR:HG23	2.52	0.45
1:A:193:ILE:HG23	1:A:292:PHE:CE2	2.51	0.44
2:B:283:PHE:CD2	2:B:324:LEU:HB3	2.52	0.44
2:B:306:GLY:C	2:B:308:THR:H	2.25	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
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
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
5:E:53:VAL:HG13	5:E:54:PHE:N	2.33	0.44
6:F:163:GLU:O	6:F:167:ASN:ND2	2.50	0.44
7:G:110:ILE:CD1	7:G:128:TRP:HB3	2.47	0.44
1:A:243:ASN:O	1:A:244:LYS:C	2.61	0.44
4:D:75:LEU:HD23	4:D:75:LEU:C	2.41	0.44
5:E:20:ALA:O	5:E:22:LEU:HD22	2.18	0.44
5:E:113:LEU:C	5:E:115:ALA:H	2.25	0.44
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.99	0.44
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.53	0.44
1:A:205:GLN:CD	1:A:209:ARG:HH22	2.26	0.44
5:E:24:ILE:O	5:E:24:ILE:HG12	2.15	0.44
1:A:25:THR:HG22	1:A:26:GLU:HG2	2.00	0.43
3:C:183:THR:HG21	3:C:185:TRP:HD1	1.83	0.43
4:D:189:ARG:HA	4:D:192:SER:O	2.18	0.43
5:E:56:LYS:NZ	5:E:170:ASN:OD1	2.50	0.43
1:A:232:SER:HA	1:A:275:ARG:O	2.18	0.43
1:A:309:ILE:HA	1:A:312:ARG:NE	2.20	0.43
2:B:185:ALA:O	2:B:186:GLY:C	2.61	0.43
4:D:131:PHE:CD1	4:D:139:GLU:HG3	2.53	0.43
1:A:117:LEU:HD13	1:A:190:ILE:HD12	2.00	0.43
1:A:143:VAL:HG13	1:A:146:VAL:CG2	2.48	0.43
1:A:172:ASP:HB2	9:A:501:ADP:O5'	2.18	0.43
1:A:295:PRO:HD2	1:A:298:GLU:CD	2.43	0.43
1:A:343:VAL:HG23	1:A:346:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:HIS:CD2	2:B:177:HIS:H	2.36	0.43
2:B:322:LYS:HG3	2:B:340:PHE:CZ	2.52	0.43
3:C:74:ARG:HG2	3:C:97:ARG:O	2.18	0.43
3:C:126:GLU:C	3:C:128:GLU:H	2.26	0.43
3:C:327:ASN:HB2	3:C:351:ASP:HB3	1.99	0.43
4:D:207:LEU:HA	4:D:210:LYS:HG3	2.00	0.43
6:F:25:PHE:CD1	6:F:67:ILE:HD13	2.53	0.43
7:G:39:GLU:HG2	7:G:78:ILE:HD13	2.01	0.43
3:C:259:VAL:HG12	3:C:332:ILE:CD1	2.49	0.43
4:D:75:LEU:HD13	4:D:123:SER:N	2.34	0.43
4:D:265:ARG:NH1	6:F:145:GLU:OE2	2.51	0.43
7:G:110:ILE:HD11	7:G:128:TRP:HB3	1.99	0.43
3:C:17:ASN:ND2	3:C:22:GLN:HG3	2.33	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
1:A:347:LEU:HD22	1:A:363:ILE:HD12	2.01	0.43
2:B:153:THR:HG22	2:B:153:THR:O	2.17	0.43
2:B:178:LEU:HD21	2:B:288:ALA:O	2.17	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
2:B:141:GLN:HE21	2:B:141:GLN:HB3	1.65	0.43
4:D:234:ALA:HB2	4:D:237:ARG:NH1	2.34	0.43
5:E:15:LEU:HD22	5:E:63:GLU:HG3	1.97	0.43
3:C:96:ASN:C	3:C:97:ARG:HD3	2.42	0.43
3:C:360:ARG:HA	3:C:363:GLU:OE1	2.18	0.43
4:D:262:ILE:HG22	4:D:266:MET:HE2	1.99	0.43
3:C:269:LEU:HB3	3:C:283:GLY:HA2	2.01	0.43
5:E:8:LEU:HD12	5:E:41:ILE:CD1	2.48	0.43
6:F:60:LYS:H	6:F:75:ALA:HB3	1.84	0.43
1:A:60:PHE:CE1	1:A:95:GLN:NE2	2.87	0.43
1:A:147:LEU:HD12	1:A:377:VAL:HG13	2.01	0.43
3:C:102:VAL:O	3:C:103:ARG:HG2	2.18	0.43
3:C:102:VAL:O	3:C:103:ARG:NH1	2.50	0.43
5:E:133:LEU:HB3	5:E:137:ARG:HH12	1.84	0.43
1:A:143:VAL:HG13	1:A:146:VAL:HG23	2.00	0.42
1:A:259:ILE:CD1	1:A:266:GLU:HG3	2.48	0.42
4:D:15:LEU:HA	4:D:15:LEU:HD23	1.81	0.42
7:G:21:GLU:CD	7:G:21:GLU:C	2.87	0.42
7:G:68:SER:O	7:G:71:VAL:CG1	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLU:HG2	9:B:395:ADP:C4	2.54	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
4:D:23:ALA:C	4:D:25:GLY:H	2.26	0.42
5:E:157:SER:C	5:E:159:TRP:N	2.76	0.42
7:G:99:ASP:O	7:G:102:GLY:N	2.52	0.42
1:A:17:THR:HG22	1:A:19:LEU:HD23	2.01	0.42
1:A:230:ARG:HB3	1:A:230:ARG:NH1	2.31	0.42
3:C:30:HIS:HB3	3:C:51:HIS:O	2.20	0.42
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
5:E:78:CYS:SG	5:E:95:MET:HE2	2.59	0.42
6:F:45:GLU:HB3	7:G:24:PHE:CE2	2.54	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
3:C:201:SER:HB3	7:G:149:LYS:HZ2	1.82	0.42
3:C:254:THR:HA	3:C:340:ALA:O	2.19	0.42
4:D:130:GLN:OE1	4:D:130:GLN:HA	2.19	0.42
5:E:86:ASN:C	5:E:154:ASP:HA	2.44	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
2:B:219:LYS:HG2	2:B:220:LEU:CD1	2.48	0.42
3:C:107:ASN:ND2	3:C:109:LYS:N	2.57	0.42
6:F:2:THR:C	6:F:4:THR:N	2.75	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
5:E:93:LYS:C	5:E:95:MET:N	2.75	0.42
5:E:153:ASN:HD22	5:E:153:ASN:HA	1.64	0.42
4:D:223:ILE:N	4:D:223:ILE:CD1	2.81	0.42
1:A:328:PHE:CZ	9:A:501:ADP:H2	2.37	0.42
2:B:165:HIS:CD2	2:B:181:ARG:HE	2.37	0.42
2:B:335:GLU:O	2:B:336:LYS:C	2.63	0.42
3:C:111:PHE:CD1	3:C:111:PHE:C	2.96	0.42
5:E:78:CYS:HA	5:E:95:MET:HE1	2.01	0.42
1:A:153:TRP:CE3	1:A:161:ARG:HD3	2.53	0.42
1:A:238:LEU:HD21	1:A:280:GLU:HG2	2.02	0.42
1:A:279:PRO:HG3	1:A:328:PHE:CE1	2.54	0.42
3:C:366:LEU:HD12	3:C:366:LEU:N	2.35	0.42
4:D:137:GLU:CD	4:D:158:LYS:HE2	2.45	0.42
5:E:113:LEU:HD11	5:E:169:MET:CE	2.50	0.42
5:E:144:LEU:HD23	5:E:144:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:HIS:N	1:A:285:PRO:HD3	2.35	0.42
1:A:308:PRO:CG	2:B:207:SER:HB2	2.49	0.42
1:A:360:PRO:O	1:A:361:LYS:C	2.62	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
4:D:213:ASP:OD1	4:D:213:ASP:N	2.51	0.42
5:E:5:HIS:HD2	5:E:65:ASP:OD2	2.03	0.42
1:A:113:THR:HA	1:A:142:ALA:O	2.20	0.41
3:C:47:GLU:HG2	3:C:49:LYS:HE3	2.01	0.41
4:D:189:ARG:C	4:D:191:ALA:N	2.78	0.41
4:D:239:ASN:HA	4:D:242:ASN:HD22	1.85	0.41
5:E:112:PRO:HB2	5:E:171:LYS:HD2	2.02	0.41
1:A:64:ASP:C	1:A:66:ALA:H	2.28	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
6:F:91:MET:HB3	6:F:95:MET:HE2	2.01	0.41
1:A:78:ILE:C	1:A:79:ARG:HD2	2.45	0.41
2:B:286:ILE:HD12	2:B:298:TYR:CE2	2.56	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
1:A:163:LEU:HG	1:A:416:VAL:HG13	2.03	0.41
1:A:335:LEU:HD23	1:A:335:LEU:O	2.19	0.41
4:D:60:SER:HB2	4:D:91:TYR:HA	2.02	0.41
5:E:18:ASN:ND2	5:E:118:ALA:H	2.18	0.41
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.88	0.41
1:A:62:ILE:HD11	1:A:100:TYR:HE2	1.83	0.41
1:A:116:PRO:HG2	1:A:178:ILE:HD13	2.01	0.41
1:A:169:ASP:HA	1:A:322:SER:O	2.21	0.41
2:B:290:ASP:O	2:B:293:THR:N	2.53	0.41
3:C:183:THR:CG2	3:C:184:PRO:N	2.83	0.41
4:D:274:LEU:HD23	4:D:274:LEU:HA	1.89	0.41
5:E:8:LEU:HD11	5:E:41:ILE:HA	2.02	0.41
1:A:36:ALA:HB1	1:A:72:TYR:HB3	2.01	0.41
2:B:323:GLN:HG2	7:G:14:VAL:HG13	2.03	0.41
4:D:171:ASP:HB3	4:D:174:ASP:CG	2.46	0.41
5:E:42:VAL:HA	5:E:71:ILE:HD13	2.03	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
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
3:C:332:ILE:O	3:C:332:ILE:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:ALA:C	3:C:366:LEU:HD12	2.45	0.41
4:D:77:LYS:HA	4:D:77:LYS:HD2	1.80	0.41
6:F:125:GLN:HE21	6:F:125:GLN:CA	2.30	0.41
1:A:5:LEU:HB3	1:A:108:HIS:CE1	2.56	0.41
1:A:283:PHE:C	1:A:285:PRO:HD3	2.46	0.41
1:A:313:ARG:HB2	1:A:314:PRO:HD3	2.03	0.41
1:A:400:TYR:CE1	1:A:405:PRO:HB3	2.55	0.41
2:B:161:ASP:HB2	9:B:395:ADP:H3'	2.02	0.41
2:B:166:ILE:O	2:B:168:PRO:HD3	2.20	0.41
2:B:326:LEU:HD23	2:B:327:GLU:N	2.36	0.41
9:B:395:ADP:O1B	9:B:395:ADP:O1A	2.38	0.41
3:C:358:ASP:HB3	3:C:361:SER:HB3	2.01	0.41
4:D:35:PHE:CD2	4:D:35:PHE:N	2.88	0.41
4:D:54:LYS:HD2	4:D:54:LYS:N	2.34	0.41
6:F:4:THR:CG2	6:F:55:ARG:HE	2.31	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
4:D:263:HIS:HD2	4:D:266:MET:HE3	1.83	0.41
4:D:278:ASN:C	4:D:280:ALA:N	2.75	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
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
3:C:90:LEU:HD23	3:C:90:LEU:C	2.42	0.40
4:D:59:ILE:HB	4:D:116:LEU:HD13	2.02	0.40
4:D:201:SER:OG	4:D:204:GLU:O	2.32	0.40
7:G:66:THR:HB	7:G:71:VAL:HG11	2.01	0.40
1:A:195:ILE:HA	1:A:199:ASP:OD2	2.21	0.40
1:A:205:GLN:CD	1:A:209:ARG:NH2	2.79	0.40
3:C:144:THR:CB	6:F:28:GLN:HE21	2.33	0.40
4:D:220:ILE:N	4:D:220:ILE:HD12	2.36	0.40
6:F:4:THR:C	6:F:7:PRO:HD2	2.46	0.40
1:A:158:VAL:O	1:A:158:VAL:HG23	2.22	0.40
2:B:147:TYR:O	2:B:151:LEU:O	2.39	0.40
3:C:7:LEU:CD1	3:C:27:PRO:HB2	2.52	0.40
4:D:237:ARG:O	4:D:241:ILE:HG13	2.22	0.40
7:G:60:LYS:O	7:G:61:ASN:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/418 (93%)	347 (89%)	36 (9%)	6 (2%)	8	18
2	B	201/394 (51%)	164 (82%)	24 (12%)	13 (6%)	1	1
3	C	337/372 (91%)	297 (88%)	34 (10%)	6 (2%)	6	15
4	D	281/300 (94%)	255 (91%)	24 (8%)	2 (1%)	18	35
5	E	169/178 (95%)	136 (80%)	25 (15%)	8 (5%)	2	3
6	F	165/168 (98%)	156 (94%)	8 (5%)	1 (1%)	21	38
7	G	128/151 (85%)	115 (90%)	10 (8%)	3 (2%)	5	11
All	All	1670/1981 (84%)	1470 (88%)	161 (10%)	39 (2%)	5	11

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	329 (95%)	18 (5%)	21	43
2	B	164/345 (48%)	155 (94%)	9 (6%)	19	41
3	C	290/313 (93%)	280 (97%)	10 (3%)	32	58
4	D	249/264 (94%)	239 (96%)	10 (4%)	28	53
5	E	155/159 (98%)	147 (95%)	8 (5%)	21	43
6	F	154/155 (99%)	149 (97%)	5 (3%)	34	59
7	G	110/124 (89%)	100 (91%)	10 (9%)	9	19
All	All	1469/1723 (85%)	1399 (95%)	70 (5%)	23	46

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	143	VAL
1	A	160	GLU
1	A	182	GLU
1	A	195	ILE
1	A	230	ARG
1	A	239	VAL
1	A	335	LEU
1	A	353	LEU
1	A	359	LYS
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	184	ILE
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	321	LEU
3	C	324	LEU
3	C	369	LEU
3	C	372	VAL
4	D	49	ASN
4	D	108	SER
4	D	116	LEU
4	D	117	LYS
4	D	141	ARG

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Mol	Chain	Res	Type
4	D	202	HIS
4	D	203	ARG
4	D	223	ILE
4	D	265	ARG
4	D	277	LEU
5	E	24	ILE
5	E	39	THR
5	E	63	GLU
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	104	LEU
6	F	165	LEU
7	G	19	TYR
7	G	21	GLU
7	G	39	GLU
7	G	43	ASP
7	G	64	ILE
7	G	71	VAL
7	G	90	ASP
7	G	93	LYS
7	G	112	LYS
7	G	151	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) 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	255	GLN
1	A	289	ASN
1	A	318	ASN
1	A	370	HIS
1	A	395	HIS
1	A	410	HIS

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Mol	Chain	Res	Type
1	A	411	ASN
2	B	141	GLN
2	B	205	ASN
2	B	267	GLN
2	B	284	ASN
2	B	323	GLN
3	C	22	GLN
3	C	46	HIS
3	C	54	GLN
3	C	107	ASN
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	120	ASN
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 oligosaccharides 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	B	395	-	28,29,29	1.55	5 (17%)	43,45,45	1.79	9 (20%)
9	ADP	A	501	-	28,29,29	1.55	6 (21%)	43,45,45	1.84	10 (23%)

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	B	395	-	-	1/16/32/32	0/3/3/3
9	ADP	A	501	-	-	5/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	501	ADP	C2-N1	3.86	1.40	1.33
9	B	395	ADP	C2-N1	3.83	1.40	1.33
9	A	501	ADP	PB-O1B	3.55	1.61	1.50
9	B	395	ADP	PB-O1B	3.54	1.61	1.50
9	B	395	ADP	C5-N7	-3.07	1.33	1.39
9	A	501	ADP	C5-N7	-3.02	1.33	1.39
9	B	395	ADP	C8-N9	-2.43	1.33	1.37
9	A	501	ADP	C8-N9	-2.27	1.33	1.37
9	A	501	ADP	PA-O3A	2.17	1.61	1.59
9	A	501	ADP	C4-N9	-2.16	1.33	1.37
9	B	395	ADP	C4-N9	-2.14	1.33	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	395	ADP	N3-C2-N1	-5.55	120.17	128.58
9	A	501	ADP	N3-C2-N1	-5.49	120.27	128.58
9	A	501	ADP	C5-C4-N3	-4.29	120.80	126.72
9	B	395	ADP	C5-C4-N3	-4.13	121.03	126.72
9	A	501	ADP	C2-N3-C4	4.12	121.88	111.83
9	B	395	ADP	C2-N3-C4	4.07	121.78	111.83
9	B	395	ADP	N9-C8-N7	-3.24	109.34	113.94
9	A	501	ADP	N9-C8-N7	-3.15	109.47	113.94
9	A	501	ADP	C4-C5-N7	-3.07	107.07	110.58
9	A	501	ADP	C5-N7-C8	2.99	108.15	103.45
9	B	395	ADP	N3-C4-N9	2.94	132.17	127.17
9	B	395	ADP	C5-N7-C8	2.87	107.96	103.45
9	A	501	ADP	N3-C4-N9	2.85	132.01	127.17
9	B	395	ADP	C4-C5-N7	-2.81	107.37	110.58
9	B	395	ADP	O3B-PB-O3A	2.71	113.73	104.64
9	B	395	ADP	C4-N9-C8	2.66	108.53	105.74
9	A	501	ADP	O4'-C1'-C2'	-2.55	101.15	106.62
9	A	501	ADP	O3B-PB-O3A	2.53	113.13	104.64
9	A	501	ADP	C4-N9-C8	2.28	108.13	105.74

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	501	ADP	C5'-O5'-PA-O2A
9	A	501	ADP	PB-O3A-PA-O1A
9	A	501	ADP	C5'-O5'-PA-O1A
9	A	501	ADP	C5'-O5'-PA-O3A
9	A	501	ADP	PB-O3A-PA-O2A
9	B	395	ADP	PA-O3A-PB-O3B

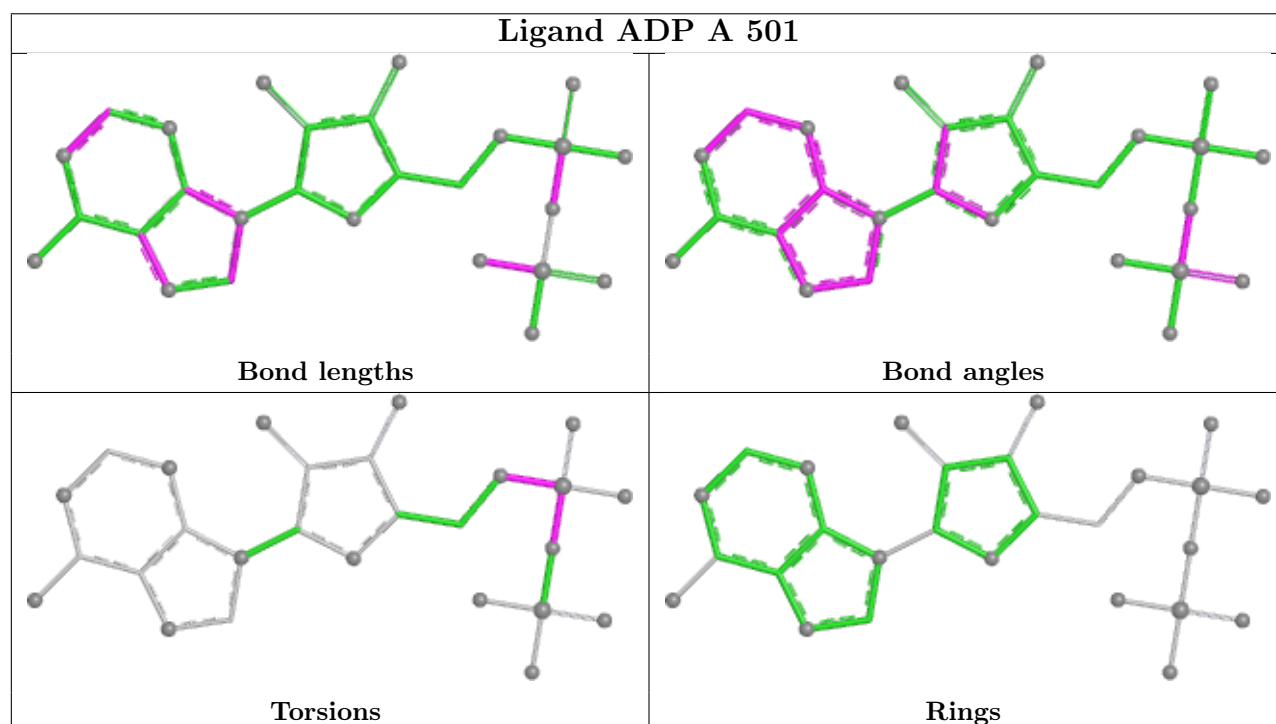
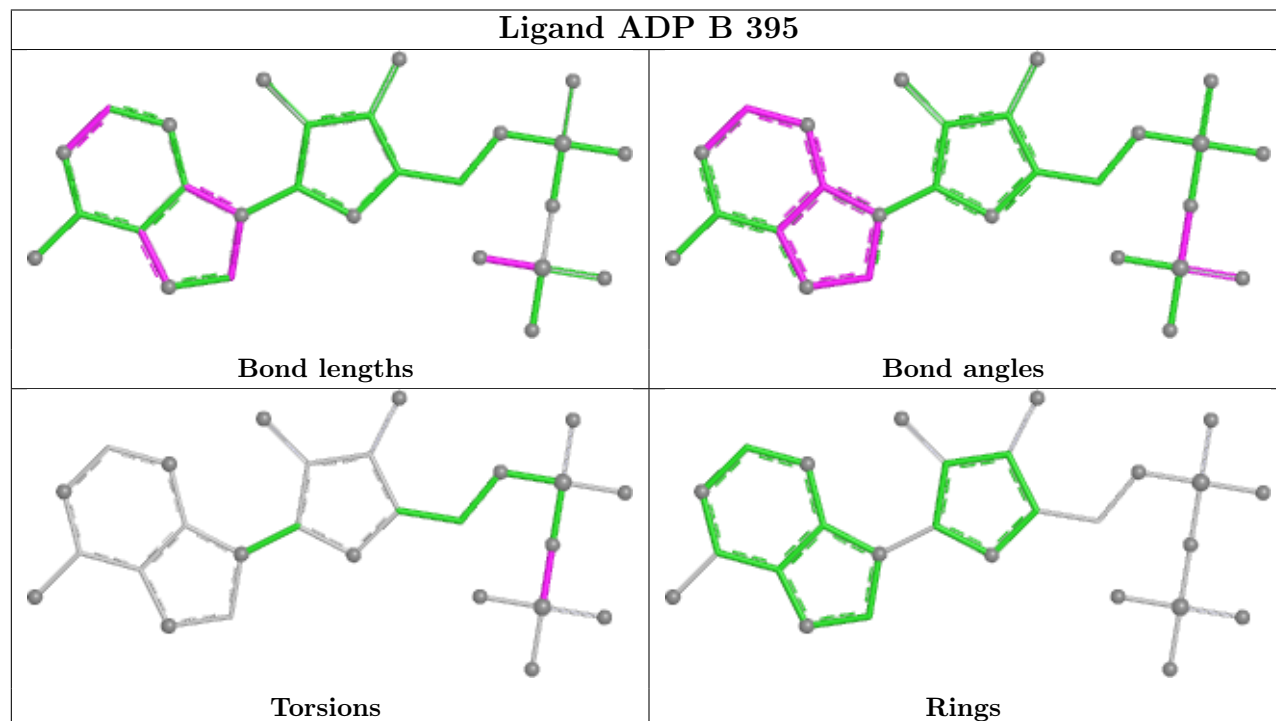
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	395	ADP	8	0
9	A	501	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/418 (94%)	0.16	17 (4%) 40 31	21, 48, 87, 109	0
2	B	203/394 (51%)	0.61	21 (10%) 12 10	29, 62, 101, 113	0
3	C	341/372 (91%)	-0.06	2 (0%) 85 82	27, 44, 71, 92	0
4	D	283/300 (94%)	-0.18	2 (0%) 84 80	25, 42, 66, 92	0
5	E	173/178 (97%)	0.49	6 (3%) 47 37	44, 60, 86, 99	0
6	F	167/168 (99%)	-0.41	1 (0%) 85 82	25, 36, 48, 75	0
7	G	134/151 (88%)	0.61	11 (8%) 17 13	36, 67, 86, 94	0
All	All	1698/1981 (85%)	0.13	60 (3%) 47 37	21, 47, 87, 113	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	343	ARG	6.7
7	G	9	ALA	4.3
2	B	334	VAL	4.1
2	B	337	LEU	4.0
5	E	175	GLY	4.0
2	B	340	PHE	3.9
1	A	262	ILE	3.9
2	B	174	SER	3.8
7	G	121	SER	3.7
5	E	96	TYR	3.6
1	A	354	SER	3.5
1	A	68	GLU	3.5
7	G	35	ALA	3.5
2	B	173	PHE	3.4
1	A	158	VAL	3.3
2	B	332	GLY	3.2
7	G	81	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	261	ALA	3.1
1	A	416	VAL	3.1
6	F	2	THR	2.8
2	B	336	LYS	2.7
2	B	331	LYS	2.7
7	G	119	ASP	2.7
2	B	146	LEU	2.7
2	B	151	LEU	2.7
7	G	19	TYR	2.7
1	A	81	GLY	2.7
2	B	143	VAL	2.6
1	A	2	ALA	2.6
5	E	35	GLU	2.5
1	A	264	LYS	2.5
7	G	150	THR	2.4
4	D	25	GLY	2.4
2	B	333	ASP	2.4
2	B	291	ILE	2.4
5	E	154	ASP	2.4
2	B	177	HIS	2.3
1	A	265	LYS	2.3
2	B	206	HIS	2.3
7	G	64	ILE	2.3
1	A	360	PRO	2.3
2	B	163	VAL	2.3
1	A	159	GLY	2.2
3	C	127	GLN	2.2
4	D	211	ASP	2.2
5	E	151	PRO	2.2
1	A	330	ASP	2.2
2	B	339	LYS	2.2
5	E	27	GLN	2.1
7	G	77	SER	2.1
1	A	80	HIS	2.1
2	B	335	GLU	2.1
7	G	115	GLU	2.1
1	A	371	HIS	2.1
2	B	172	GLY	2.1
1	A	213	VAL	2.1
7	G	37	PRO	2.1
3	C	319	ALA	2.0
1	A	414	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	254	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

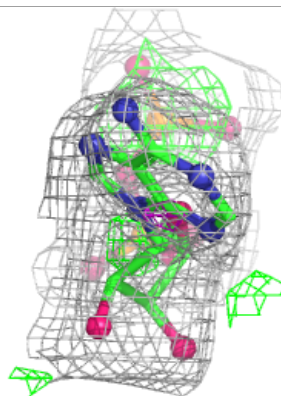
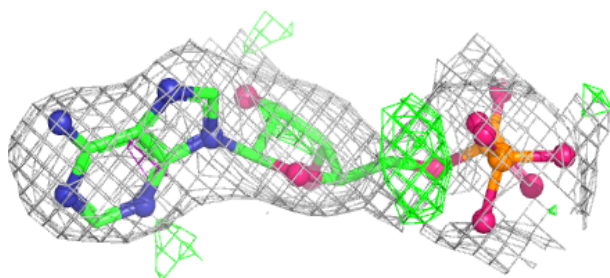
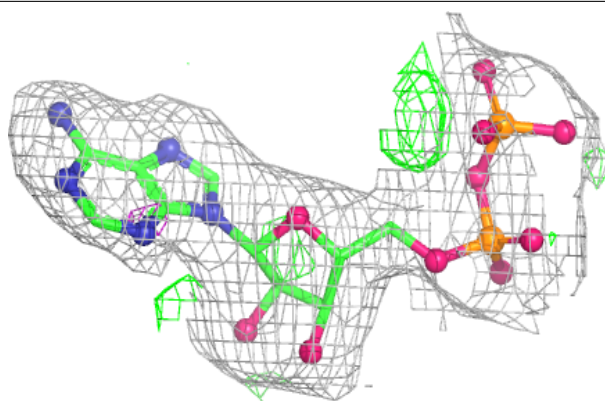
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	ADP	A	501	27/27	0.83	0.15	55,64,95,96	0
9	ADP	B	395	27/27	0.88	0.11	54,60,74,76	0
8	CA	A	500	1/1	0.95	0.12	68,68,68,68	0

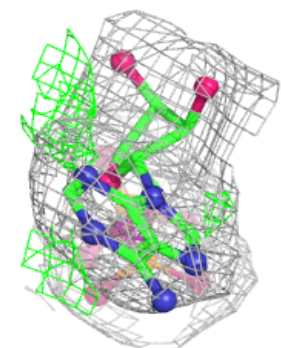
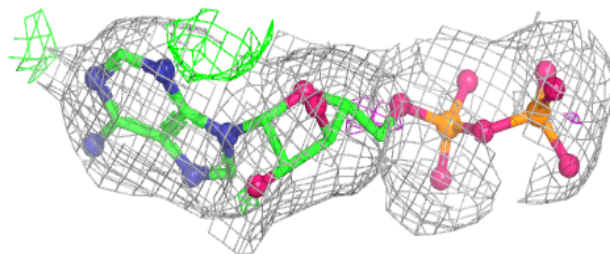
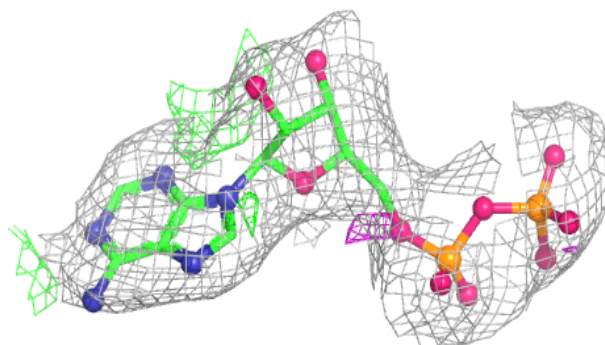
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 501:

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

**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.