



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:25 PM UTC

PDB ID : 2P9P / pdb_00002p9p
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

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

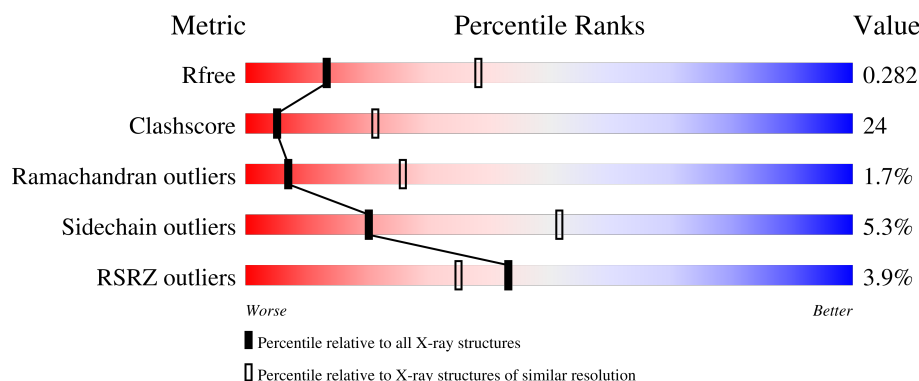
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	
2	B	394	
3	C	372	
4	D	300	
5	E	178	

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Mol	Chain	Length	Quality of chain
6	F	168	% 53% 40%
7	G	151	9% 43% 32% 10% 15%

2 Entry composition

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			

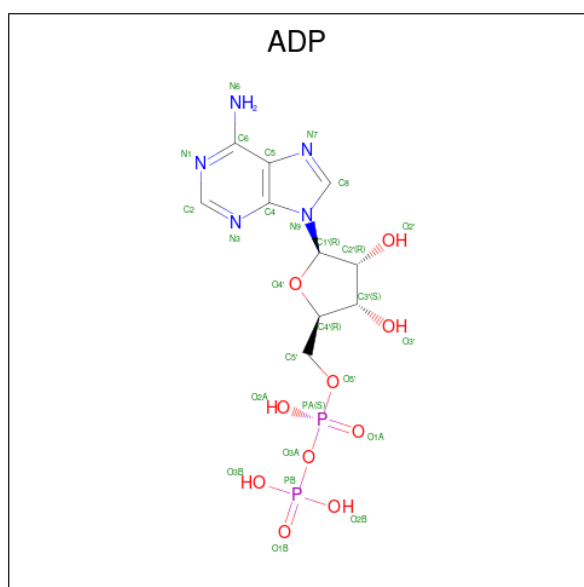
There are 2 discrepancies between the modelled and reference sequences:

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 (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).

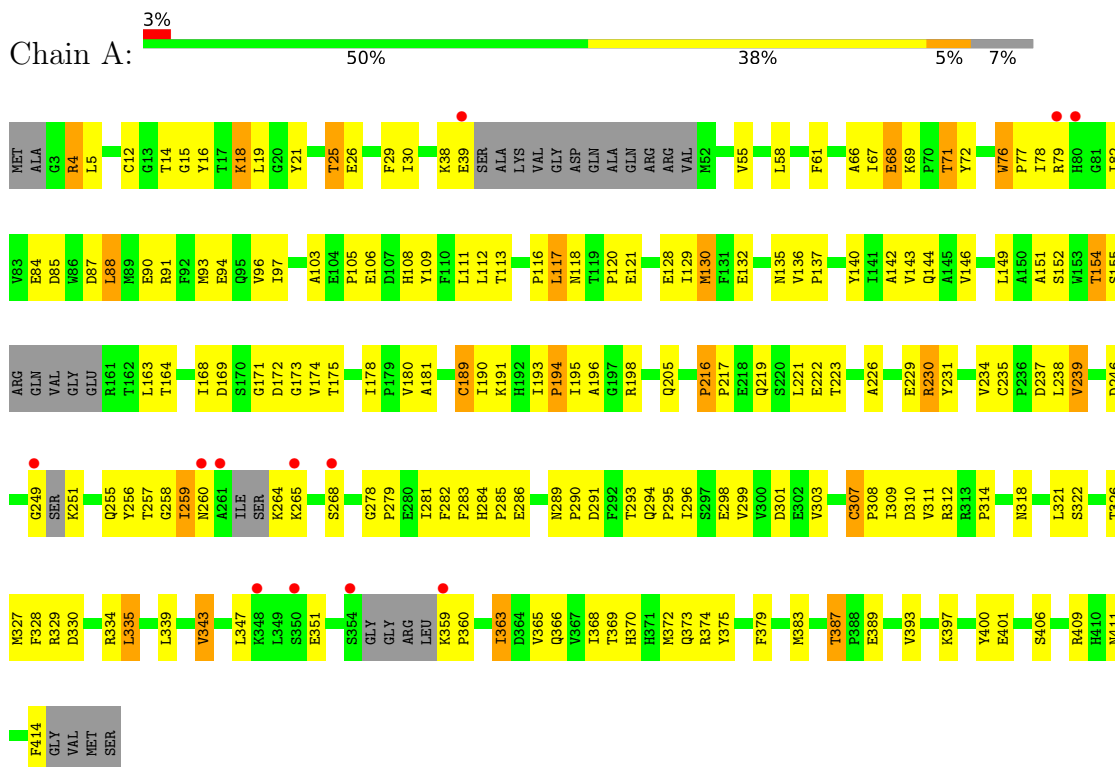


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

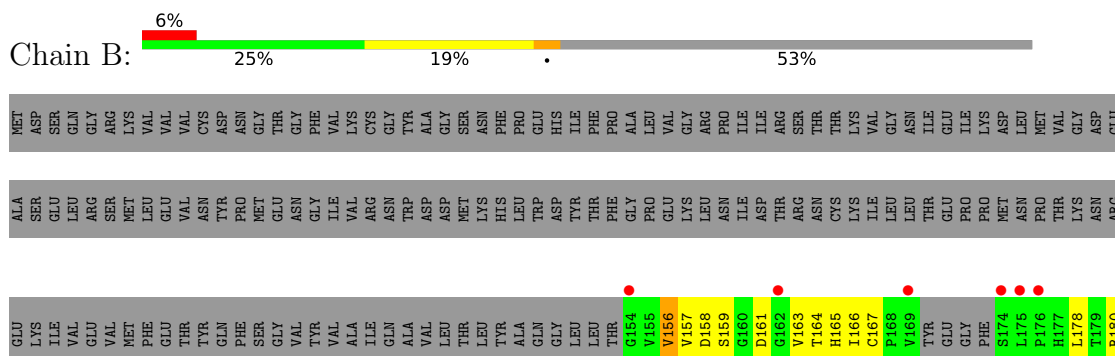
3 Residue-property plots [i](#)

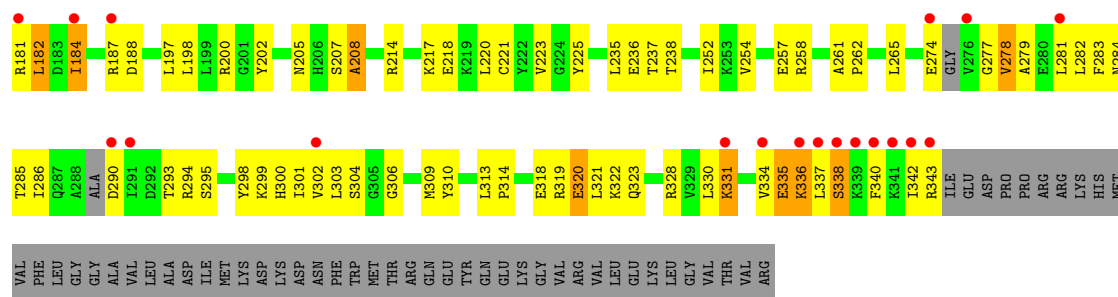
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

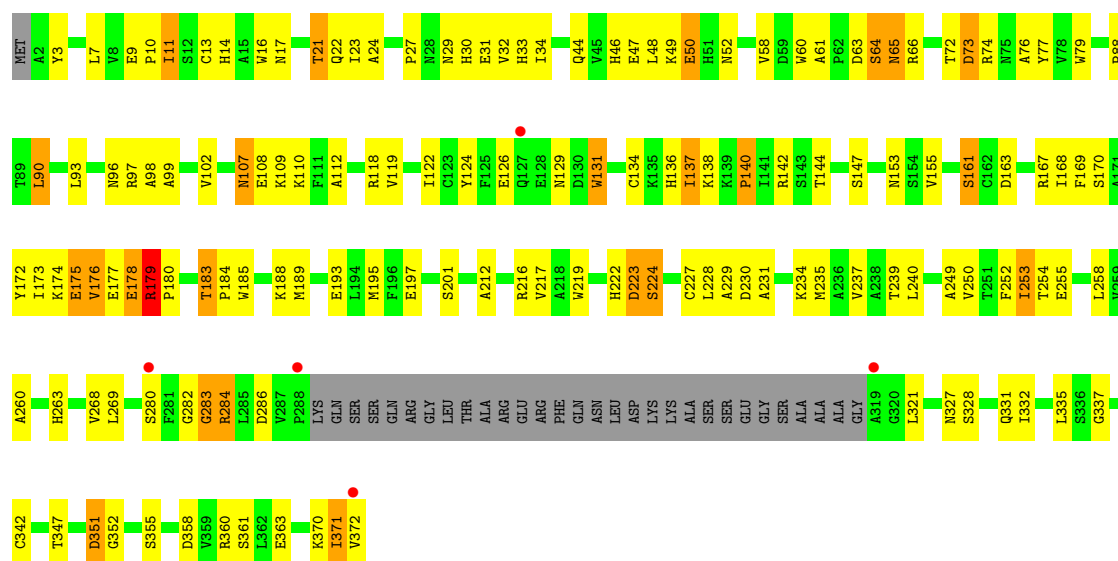


• Molecule 2: Actin-like protein 2

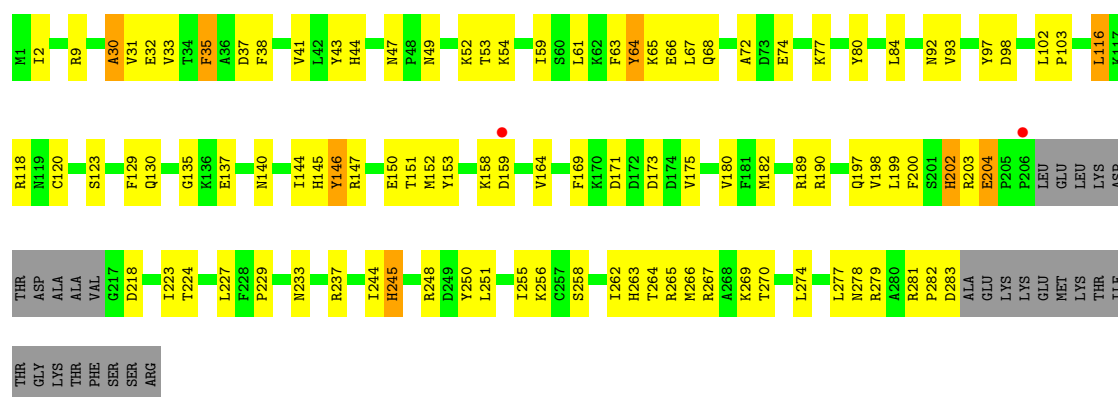




• Molecule 3: Actin-related protein 2/3 complex subunit 1B

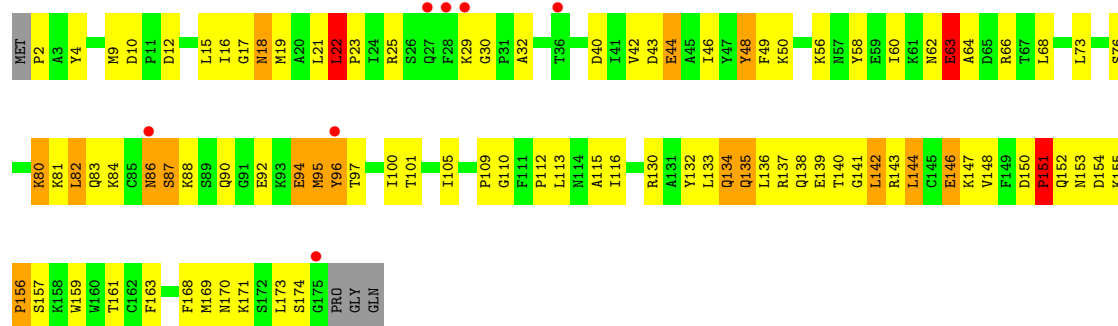


• Molecule 4: Actin-related protein 2/3 complex subunit 2

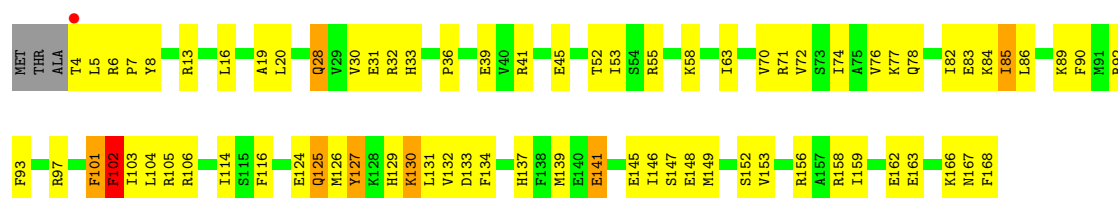


• Molecule 5: Actin-related protein 2/3 complex subunit 3

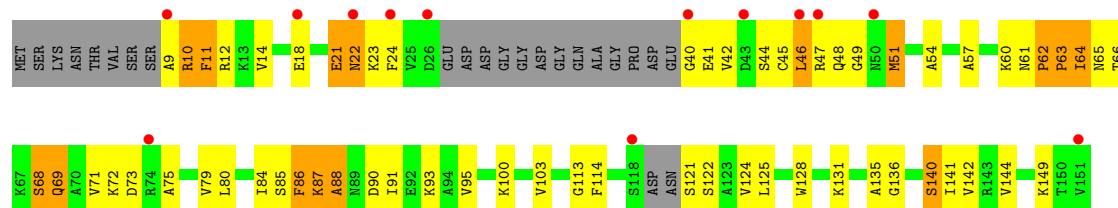
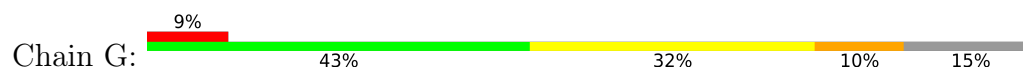




- Molecule 6: Actin-related protein 2/3 complex subunit 4



- 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	110.97Å 128.93Å 202.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.4 (50.00-2.90) 82.6 (50.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.288 0.233 , 0.282	Depositor DCC
R_{free} test set	2896 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13192	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.57	1/3156 (0.0%)	1.05	24/4287 (0.6%)
2	B	0.52	0/1473	0.95	3/1986 (0.2%)
3	C	0.53	0/2717	1.05	13/3688 (0.4%)
4	D	0.51	0/2261	0.95	8/3050 (0.3%)
5	E	0.48	0/1440	1.10	16/1943 (0.8%)
6	F	0.53	0/1381	0.99	4/1851 (0.2%)
7	G	0.45	0/992	0.98	4/1331 (0.3%)
All	All	0.52	1/13420 (0.0%)	1.02	72/18136 (0.4%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	LYS	CA-CB	5.78	1.62	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	283	GLY	N-CA-C	10.96	129.73	112.31
1	A	373	GLN	N-CA-C	9.71	121.86	111.28
5	E	174	SER	N-CA-C	-7.66	103.91	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	96	TYR	N-CA-C	-7.24	103.33	111.07
4	D	279	ARG	N-CA-C	-7.02	104.72	113.28
2	B	208	ALA	N-CA-C	6.93	118.84	111.28
5	E	49	PHE	N-CA-C	6.90	119.39	111.11
5	E	109	PRO	N-CA-C	-6.80	100.51	111.19
3	C	223	ASP	N-CA-C	-6.73	105.47	113.21
1	A	193	ILE	CA-C-N	6.61	128.11	119.84
1	A	193	ILE	C-N-CA	6.61	128.11	119.84
1	A	178	ILE	N-CA-C	6.55	114.61	107.60
3	C	30	HIS	N-CA-C	-6.55	104.92	113.17
5	E	63	GLU	N-CA-C	-6.55	105.15	113.01
4	D	9	ARG	N-CA-C	6.36	119.02	111.71
7	G	140	SER	N-CA-C	-6.28	104.53	111.82
5	E	22	LEU	CA-C-N	6.27	126.24	119.78
5	E	22	LEU	C-N-CA	6.27	126.24	119.78
1	A	326	THR	N-CA-C	-6.17	105.55	114.12
3	C	163	ASP	N-CA-C	-6.11	105.40	112.92
5	E	19	MET	N-CA-C	-6.04	102.74	110.53
4	D	80	TYR	N-CA-C	6.04	119.11	111.69
1	A	136	VAL	CA-C-N	6.00	125.70	119.64
1	A	136	VAL	C-N-CA	6.00	125.70	119.64
1	A	238	LEU	N-CA-C	5.98	117.48	110.97
1	A	130	MET	N-CA-C	5.96	117.78	111.28
6	F	28	GLN	N-CA-C	-5.96	106.14	113.41
2	B	178	LEU	N-CA-C	5.89	120.46	113.28
5	E	17	GLY	N-CA-C	-5.87	106.27	111.67
3	C	99	ALA	N-CA-C	-5.86	101.85	110.52
7	G	69	GLN	N-CA-C	-5.85	104.98	111.71
4	D	190	ARG	N-CA-C	-5.82	106.16	113.20
3	C	147	SER	N-CA-C	5.81	118.02	109.24
3	C	11	ILE	N-CA-C	-5.80	98.62	106.85
5	E	173	LEU	N-CA-C	-5.79	106.17	113.18
7	G	62	PRO	CA-C-N	5.74	127.02	119.84
7	G	62	PRO	C-N-CA	5.74	127.02	119.84
1	A	368	ILE	N-CA-C	5.73	116.45	108.89
5	E	134	GLN	N-CA-C	-5.68	106.51	113.50
1	A	109	TYR	N-CA-C	-5.68	102.08	110.48
5	E	86	ASN	N-CA-C	5.60	122.74	110.80
4	D	123	SER	N-CA-C	5.59	117.37	111.28
1	A	351	GLU	N-CA-C	-5.55	104.25	111.02
3	C	161	SER	N-CA-C	5.53	115.58	108.34
3	C	137	ILE	N-CA-C	-5.52	97.97	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	102	PHE	N-CA-C	5.51	122.54	110.80
1	A	259	ILE	N-CA-C	5.51	115.80	107.75
1	A	67	ILE	N-CA-C	5.42	115.62	110.53
1	A	231	TYR	N-CA-C	5.39	120.72	114.04
1	A	68	GLU	N-CA-C	5.35	116.86	110.44
4	D	64	TYR	N-CA-C	5.29	118.20	111.69
1	A	387	THR	CA-C-N	5.29	124.61	118.85
1	A	387	THR	C-N-CA	5.29	124.61	118.85
1	A	76	TRP	CA-C-N	5.27	126.42	119.84
1	A	76	TRP	C-N-CA	5.27	126.42	119.84
5	E	156	PRO	N-CA-C	-5.23	101.70	112.47
4	D	202	HIS	N-CA-C	5.21	117.74	109.24
1	A	118	ASN	N-CA-C	-5.21	102.68	110.23
4	D	30	ALA	N-CA-C	-5.17	103.21	110.50
3	C	178	GLU	N-CA-C	5.17	116.66	108.96
1	A	189	CYS	N-CA-C	5.14	119.51	112.88
6	F	19	ALA	N-CA-C	5.13	117.77	111.82
1	A	307	CYS	CA-C-N	5.12	125.41	119.93
1	A	307	CYS	C-N-CA	5.12	125.41	119.93
5	E	135	GLN	N-CA-C	-5.09	105.38	111.03
3	C	73	ASP	N-CA-C	-5.09	107.09	113.15
5	E	110	GLY	N-CA-C	-5.06	107.99	114.37
3	C	351	ASP	N-CA-C	-5.05	106.53	113.30
5	E	18	ASN	N-CA-C	-5.05	105.92	113.89
6	F	141	GLU	N-CA-C	5.04	117.50	111.71
3	C	253	ILE	N-CA-C	-5.02	108.38	113.20
2	B	156	VAL	N-CA-C	5.00	115.05	107.75

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	151	0
2	B	1451	0	1474	79	0
3	C	2648	0	2602	131	0
4	D	2213	0	2176	90	0
5	E	1406	0	1398	95	0
6	F	1359	0	1398	69	0
7	G	982	0	1012	65	0
8	A	1	0	0	0	0
9	A	27	0	12	3	0
9	B	27	0	12	3	0
All	All	13192	0	13054	643	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 24.

All (643) 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:HA	6:F:130:LYS:HE2	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
1:A:112:LEU:HD11	1:A:130:MET:HE2	1.53	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
1:A:87:ASP:CG	4:D:264:THR:HG22	2.01	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
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:79:ARG:HA	1:A:79:ARG:NE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:49:GLY:HA2	7:G:51:MET:HE2	1.64	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:HD3	7:G:87:LYS:N	2.05	0.71
1:A:55:VAL:CG1	1:A:58:LEU:HD12	2.19	0.71
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
6:F:86:LEU:HD22	6:F:149:MET:HE3	1.72	0.71
2:B:290:ASP:HB2	2:B:293:THR:OG1	1.90	0.71
3:C:107:ASN:C	3:C:107:ASN:HD22	1.98	0.70
3:C:189:MET:HA	3:C:195:MET:HE1	1.71	0.70
5:E:92:GLU:O	5:E:96:TYR:HD1	1.73	0.70
3:C:222:HIS:C	3:C:224:SER:H	1.99	0.70
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.74	0.70
3:C:193:GLU:HB3	3:C:195:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:170:SER:HB2	3:C:195:MET:HE3	1.74	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
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
1:A:87:ASP:OD2	4:D:264:THR:HG22	1.93	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:93:MET:HE2	1:A:130:MET:HE1	1.75	0.67
1:A:120:PRO:HB3	1:A:409:ARG:HG2	1.76	0.67
3:C:201:SER:HB3	7:G:149:LYS:HZ3	1.58	0.67
1:A:289:ASN:HD22	1:A:289:ASN:C	2.01	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
1:A:311:VAL:C	1:A:314:PRO:HD2	2.19	0.66
4:D:135:GLY:O	4:D:137:GLU:HG3	1.95	0.66
4:D:262:ILE:HG22	4:D:266:MET:HE2	1.78	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
1:A:18:LYS:N	1:A:18:LYS:HD3	2.12	0.64
3:C:11:ILE:HG13	3:C:352:GLY:HA2	1.78	0.64
5:E:16:ILE:HG23	5:E:16:ILE:O	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
1:A:21:TYR:OH	1:A:103:ALA:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:A:194:PRO:C	1:A:195:ILE:HD12	2.26	0.61
3:C:13:CYS:HA	3:C:331:GLN:NE2	2.16	0.60
5:E:150:ASP:C	5:E:152:GLN:H	2.09	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:60:TRP:HE1	3:C:65:ASN:ND2	1.98	0.60
3:C:239:THR:HG22	3:C:240:LEU:N	2.15	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
7:G:62:PRO:C	7:G:64:ILE:H	2.09	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:HG3	1:A:374:ARG:HH11	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
5:E:95:MET:HE3	5:E:95:MET:HA	1.83	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
6:F:85:ILE:HD12	6:F:85:ILE:C	2.27	0.59
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
5:E:168:PHE:CE2	5:E:169:MET:HE2	2.36	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
2:B:342:ILE:O	2:B:342:ILE:HG22	2.01	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:NH1	2:B:343:ARG:HB2	2.17	0.59
3:C:212:ALA:HB3	3:C:255:GLU:OE2	2.02	0.59
1:A:4:ARG:HH11	1:A:4:ARG:HB2	1.68	0.58
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
4:D:281:ARG:C	4:D:283:ASP:H	2.11	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: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:172:ASP:O	1:A:198:ARG:HB2	2.04	0.58
1:A:55:VAL:HG12	1:A:55:VAL:O	2.04	0.58
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.39	0.58
2:B:330:LEU:O	2:B:331:LYS:HB2	2.04	0.58
4:D:203:ARG:HB3	4:D:203:ARG:NH1	2.19	0.58
3:C:144:THR:H	6:F:28:GLN:NE2	2.02	0.58
5:E:150:ASP:C	5:E:152:GLN:N	2.60	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:C	1:A:285:PRO:HD3	2.29	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:111:LEU:HD23	1:A:111:LEU:C	2.29	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
5:E:40:ASP:CG	5:E:143:ARG:HH12	2.13	0.57
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
1:A:309:ILE:HA	1:A:312:ARG:HE	1.68	0.56
7:G:80:LEU:O	7:G:84:ILE:HD13	2.05	0.56
1:A:258:GLY:C	1:A:259:ILE:HD12	2.31	0.56
7:G:23:LYS:HG2	7:G:24:PHE:N	2.14	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
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:HA	6:F:130:LYS:CE	2.30	0.56
5:E:40:ASP:O	5:E:43:ASP:HB2	2.06	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:14:HIS:HA	3:C:24:ALA:O	2.05	0.55
3:C:144:THR:O	3:C:161:SER:HB2	2.07	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:HG3	3:C:179:ARG:HH11	1.72	0.55
6:F:5:LEU:HD13	6:F:55:ARG:HH12	1.71	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
1:A:61:PHE:C	1:A:66:ALA:HB2	2.33	0.54
1:A:372:MET:HE2	1:A:379:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:126:MET:HE3	6:F:131:LEU:HD21	1.89	0.54
6:F:158:ARG:O	6:F:162:GLU:HG3	2.07	0.54
2:B:180:ARG:CB	2:B:281:LEU:HD21	2.37	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
3:C:7:LEU:N	3:C:7:LEU:HD23	2.23	0.54
3:C:72:THR:HA	3:C:98:ALA:HB1	1.90	0.54
3:C:140:PRO:HG2	3:C:167:ARG:HE	1.73	0.54
3:C:172:TYR:C	3:C:172:TYR:CD2	2.86	0.54
2:B:335:GLU:O	2:B:336:LYS:C	2.49	0.54
5:E:76:SER:O	5:E:80:LYS:HD3	2.08	0.54
1:A:383:MET:HA	1:A:383:MET:HE2	1.91	0.53
3:C:131:TRP:HE3	3:C:131:TRP:O	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
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:N	4:D:199:LEU:HD12	2.24	0.53
5:E:112:PRO:HB2	5:E:171:LYS:HD2	1.91	0.53
5:E:140:THR:O	5:E:144:LEU:HB2	2.09	0.53
7:G:46:LEU:C	7:G:48:GLN:H	2.16	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
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:222:HIS:C	3:C:224:SER:N	2.67	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:HE2	6:F:58:LYS:HA	1.90	0.53
6:F:71:ARG:HA	6:F:116:PHE:O	2.08	0.53
6:F:163:GLU:O	6:F:167:ASN:ND2	2.42	0.53
4:D:74:GLU:OE1	4:D:74:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ASP:C	3:C:65:ASN:H	2.16	0.52
3:C:126:GLU:CB	3:C:131:TRP:HZ3	2.19	0.52
4:D:248:ARG:O	4:D:248:ARG:HD3	2.09	0.52
3:C:102:VAL:HA	3:C:112:ALA:O	2.08	0.52
4:D:198:VAL:C	4:D:199:LEU:HD12	2.34	0.52
1:A:39:GLU:HG3	1:A:39:GLU:O	2.08	0.52
6:F:97:ARG:HG3	6:F:97:ARG:HH11	1.73	0.52
2:B:198:LEU:C	2:B:200:ARG:N	2.66	0.52
4:D:248:ARG:HD3	4:D:248:ARG:C	2.34	0.52
1:A:151:ALA:O	1:A:154:THR:HB	2.09	0.52
3:C:178:GLU:O	3:C:179:ARG:C	2.52	0.52
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:44:GLU:HG2	5:E:48:TYR:HE2	1.75	0.52
5:E:88:LYS:N	5:E:153:ASN:ND2	2.55	0.52
2:B:331:LYS:HD3	2:B:331:LYS:C	2.35	0.52
1:A:343:VAL:O	1:A:347:LEU:HD13	2.10	0.52
3:C:96:ASN:C	3:C:97:ARG:HD3	2.35	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
5:E:82:LEU:HD23	5:E:148:VAL:HG21	1.93	0.51
7:G:87:LYS:O	7:G:88:ALA:C	2.54	0.51
7:G:149:LYS:HD3	7:G:149:LYS:N	2.25	0.51
4:D:53:THR:C	4:D:54:LYS:HD2	2.34	0.51
5:E:113:LEU:C	5:E:115:ALA:H	2.17	0.51
1:A:90:GLU:HG3	1:A:129:ILE:HG23	1.93	0.51
1:A:152:SER:C	1:A:154:THR:H	2.18	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
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:O	4:D:203:ARG:HG2	2.10	0.51
6:F:76:VAL:HG12	6:F:77:LYS:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:198:LEU:C	2:B:200:ARG:H	2.19	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
3:C:107:ASN:ND2	3:C:107:ASN:C	2.64	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:13:CYS:SG	3:C:58:VAL:HG23	2.51	0.50
3:C:131:TRP:O	3:C:131:TRP:CE3	2.64	0.50
1:A:389:GLU:CD	1:A:414:PHE:HB2	2.37	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
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: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
7:G:84:ILE:C	7:G:86:PHE:H	2.20	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: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:HG3	3:C:142:ARG:HH11	1.78	0.49
4:D:67:LEU:HD13	4:D:120:CYS:O	2.13	0.49
4:D:282:PRO:O	4:D:283:ASP:CB	2.61	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:31:GLU:HG2	3:C:49:LYS:HG2	1.95	0.49
3:C:269:LEU:H	3:C:283:GLY:CA	2.25	0.49
4:D:244:ILE:HG23	4:D:245:HIS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:281:ARG:C	4:D:283:ASP:N	2.69	0.49
6:F:30:VAL:HG11	6:F:33:HIS:CE1	2.48	0.49
2:B:237:THR:HG22	6:F:105:ARG:HG3	1.93	0.49
3:C:72:THR:C	3:C:74:ARG:H	2.20	0.49
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.43	0.49
6:F:74:ILE:HD13	6:F:139:MET:HG2	1.94	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
4:D:202:HIS:C	4:D:204:GLU:H	2.20	0.49
5:E:95:MET:HG2	5:E:141:GLY:C	2.38	0.49
1:A:309:ILE:O	1:A:312:ARG:HG3	2.14	0.48
2:B:331:LYS:HD3	2:B:331:LYS:O	2.13	0.48
5:E:156:PRO:O	5:E:157:SER:C	2.55	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:113:LEU:C	5:E:115:ALA:N	2.71	0.48
5:E:134:GLN:O	5:E:138:GLN:HG3	2.12	0.48
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
1:A:152:SER:C	1:A:154:THR:N	2.68	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
1:A:135:ASN:ND2	4:D:256:LYS:HE3	2.29	0.48
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.43	0.48
3:C:10:PRO:CG	6:F:124:GLU:HG2	2.42	0.48
3:C:201:SER:HB3	7:G:149:LYS:HZ2	1.78	0.48
4:D:244:ILE:CG2	4:D:245:HIS:N	2.77	0.48
1:A:140:TYR:CE1	1:A:411:ASN:HB3	2.49	0.48
1:A:216:PRO:O	1:A:217:PRO:C	2.56	0.48
7:G:100:LYS:NZ	7:G:135:ALA:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:PRO:HG3	3:C:33:HIS:CD2	2.49	0.47
5:E:152:GLN:HA	5:E:152:GLN:OE1	2.14	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
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
2:B:290:ASP:HB2	2:B:293:THR:HG1	1.79	0.47
3:C:52:ASN:N	3:C:73:ASP:OD2	2.44	0.47
3:C:223:ASP:OD1	3:C:223:ASP:C	2.57	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
5:E:18:ASN:ND2	5:E:66:ARG:NE	2.63	0.47
5:E:60:ILE:HD12	5:E:116:ILE:HG23	1.97	0.47
4:D:145:HIS:C	4:D:147:ARG:H	2.23	0.47
4:D:251:LEU:O	4:D:255:ILE:HG13	2.15	0.47
1:A:69:LYS:HB3	1:A:72:TYR:HD1	1.80	0.47
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
2:B:309:MET:HE3	9:B:395:ADP:N7	2.29	0.47
1:A:85:ASP:OD2	1:A:88:LEU:HD22	2.14	0.47
1:A:189:CYS:O	1:A:303:VAL:HG13	2.15	0.47
2:B:163:VAL:HG23	2:B:182:LEU:O	2.15	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: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
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
5:E:58:TYR:CD1	5:E:168:PHE:HZ	2.33	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
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:HD23	3:C:335:LEU:HA	1.76	0.46
5:E:30:GLY:C	5:E:32:ALA:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:ARG:HD3	4:D:118:ARG:C	2.41	0.46
7:G:103:VAL:HG11	7:G:136:GLY:CA	2.45	0.46
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
6:F:146:ILE:HA	6:F:149:MET:HE2	1.98	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
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.76	0.45
7:G:51:MET:HG3	7:G:87:LYS:NZ	2.31	0.45
7:G:60:LYS:O	7:G:61:ASN:C	2.59	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
2:B:322:LYS:HG2	2:B:340:PHE:CZ	2.51	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
5:E:153:ASN:CG	5:E:154:ASP:N	2.74	0.45
2:B:323:GLN:HB3	7:G:11:PHE:O	2.17	0.45
3:C:253:ILE:O	3:C:254:THR:HG23	2.16	0.45
6:F:126:MET:CE	6:F:131:LEU:HD21	2.47	0.45
6:F:130:LYS:HE2	6:F:130:LYS:CA	2.29	0.45
1:A:295:PRO:HD2	1:A:298:GLU:CD	2.41	0.44
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:29:PHE:C	1:A:30:ILE:HG13	2.42	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:81:LYS:O	5:E:82:LEU:C	2.60	0.44
7:G:87:LYS:CE	7:G:87:LYS:H	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
3:C:47:GLU:C	3:C:48:LEU:HD12	2.42	0.44
4:D:151:THR:HG22	4:D:152:MET:N	2.33	0.44
5:E:9:MET:HE1	5:E:15:LEU:HD21	1.99	0.44
7:G:41:GLU:O	7:G:44:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:ILE:O	7:G:142:VAL:C	2.60	0.44
4:D:38:PHE:O	4:D:41:VAL:HG23	2.16	0.44
7:G:64:ILE:HG22	7:G:65:ASN:CG	2.43	0.44
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.53	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
5:E:83:GLN:CD	5:E:84:LYS:HE3	2.43	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:193:GLU:CB	3:C:195:MET:HE2	2.47	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
6:F:167:ASN:C	6:F:168:PHE:O	2.59	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:37:ASP:HB2	4:D:43:TYR:CE1	2.53	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
2:B:254:VAL:HG12	2:B:258:ARG:HG3	1.99	0.43
3:C:64:SER:O	3:C:65:ASN:C	2.62	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:252:PHE:CZ	3:C:258:LEU:HD21	2.54	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
1:A:4:ARG:CG	1:A:4:ARG:NH1	2.78	0.43
1:A:321:LEU:HD12	1:A:369:THR:HG22	1.99	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
7:G:51:MET:HG3	7:G:87:LYS:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ASN:O	2:B:285:THR:C	2.61	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:HB2	2:B:343:ARG:HH11	1.84	0.43
3:C:3:TYR:CD1	3:C:3:TYR:C	2.97	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
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
4:D:64:TYR:HB3	4:D:92:ASN:ND2	2.34	0.42
5:E:142:LEU:C	5:E:144:LEU:N	2.77	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:72:VAL:HB	6:F:116:PHE:HB2	2.02	0.42
6:F:104:LEU:HD21	6:F:114:ILE:HD11	2.01	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:O	5:E:134:GLN:HG2	2.20	0.42
7:G:87:LYS:CD	7:G:87:LYS:H	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: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:93:PHE:CD2	6:F:93:PHE:C	2.97	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:77:PRO:HG3	1:A:88:LEU:HB3	2.01	0.42
1:A:283:PHE:O	1:A:295:PRO:HB3	2.19	0.42
2:B:306:GLY:HA2	2:B:309:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	5:E:130:ARG:NH1	2.35	0.42
1:A:15:GLY:O	1:A:16:TYR:CD2	2.73	0.42
1:A:38:LYS:HE2	1:A:72:TYR:CE2	2.55	0.42
1:A:298:GLU:O	1:A:301:ASP:HB3	2.20	0.42
4:D:130:GLN:OE1	4:D:130:GLN:HA	2.20	0.42
4:D:267:ARG:HG3	4:D:267:ARG:HH11	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
3:C:189:MET:HA	3:C:195:MET:CE	2.43	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
5:E:86:ASN:HB3	5:E:154:ASP:OD2	2.20	0.41
1:A:14:THR:HA	1:A:78:ILE:CG2	2.50	0.41
1:A:149:LEU:O	1:A:152:SER:OG	2.32	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
3:C:174:LYS:HE2	3:C:174:LYS:HB3	1.64	0.41
3:C:321:LEU:HD13	6:F:129:HIS:CE1	2.55	0.41
4:D:77:LYS:HA	4:D:77:LYS:HD2	1.79	0.41
4:D:265:ARG:NH2	6:F:148:GLU:HB3	2.34	0.41
5:E:135:GLN:O	5:E:136:LEU:C	2.63	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
3:C:228:LEU:C	3:C:228:LEU:HD23	2.46	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
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
2:B:254:VAL:HG13	2:B:257:GLU:CG	2.50	0.41
4:D:145:HIS:C	4:D:147:ARG:N	2.79	0.41
7:G:10:ARG:C	7:G:12:ARG:H	2.29	0.41
7:G:21:GLU:O	7:G:22:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HB2	1:A:4:ARG:NH1	2.35	0.41
1:A:108:HIS:O	1:A:137:PRO:HD2	2.20	0.41
1:A:121:GLU:H	1:A:121:GLU:CD	2.28	0.41
1:A:235:CYS:O	1:A:334:ARG:NH1	2.54	0.41
3:C:77:TYR:CE2	3:C:90:LEU:HG	2.56	0.41
1:A:155:SER:HB2	1:A:370:HIS:HB3	2.02	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
4:D:31:VAL:N	4:D:47:ASN:OD1	2.42	0.41
5:E:42:VAL:O	5:E:46:ILE:HG13	2.21	0.41
5:E:82:LEU:O	5:E:83:GLN:C	2.63	0.41
7:G:84:ILE:C	7:G:86:PHE:N	2.79	0.41
7:G:86:PHE:CG	7:G:128:TRP:HZ2	2.39	0.41
1:A:259:ILE:HD12	1:A:259:ILE:N	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
5:E:62:ASN:C	5:E:64:ALA:N	2.77	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
5:E:152:GLN:O	5:E:155:LYS:HB2	2.21	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
5:E:153:ASN:CG	5:E:154:ASP:H	2.28	0.40
6:F:13:ARG:NH1	6:F:133:ASP:OD1	2.33	0.40
7:G:62:PRO:C	7:G:64:ILE:N	2.77	0.40
1:A:79:ARG:HA	1:A:79:ARG:HE	1.77	0.40
1:A:295:PRO:O	1:A:296:ILE:C	2.64	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
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
3:C:188:LYS:O	3:C:195:MET:HE1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:LYS:HE2	4:D:65:LYS:CA	2.41	0.40
4:D:269:LYS:O	4:D:270:THR:C	2.63	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%)	24	54
2	B	176/394 (45%)	149 (85%)	22 (12%)	5 (3%)	4	15
3	C	337/372 (91%)	306 (91%)	24 (7%)	7 (2%)	5	21
4	D	269/300 (90%)	251 (93%)	17 (6%)	1 (0%)	30	59
5	E	172/178 (97%)	147 (86%)	23 (13%)	2 (1%)	10	34
6	F	163/168 (97%)	150 (92%)	9 (6%)	4 (2%)	4	17
7	G	122/151 (81%)	101 (83%)	14 (12%)	7 (6%)	1	4
All	All	1615/1981 (82%)	1449 (90%)	138 (8%)	28 (2%)	7	26

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

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Mol	Chain	Res	Type
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%)	309 (94%)	21 (6%)	16	44
2	B	157/345 (46%)	150 (96%)	7 (4%)	24	58
3	C	290/313 (93%)	280 (97%)	10 (3%)	32	66
4	D	241/264 (91%)	234 (97%)	7 (3%)	37	71
5	E	153/159 (96%)	139 (91%)	14 (9%)	8	27
6	F	153/155 (99%)	146 (95%)	7 (5%)	24	57
7	G	106/124 (86%)	96 (91%)	10 (9%)	8	26
All	All	1430/1723 (83%)	1354 (95%)	76 (5%)	20	52

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	LYS
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	230	ARG
1	A	239	VAL
1	A	255	GLN
1	A	282	PHE
1	A	310	ASP
1	A	318	ASN
1	A	335	LEU
1	A	343	VAL
1	A	363	ILE
1	A	366	GLN
1	A	387	THR
2	B	167	CYS
2	B	182	LEU
2	B	184	ILE
2	B	220	LEU
2	B	235	LEU
2	B	274	GLU
2	B	320	GLU
3	C	21	THR
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
4	D	33	VAL
4	D	35	PHE
4	D	49	ASN
4	D	116	LEU

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Mol	Chain	Res	Type
4	D	204	GLU
4	D	227	LEU
4	D	245	HIS
5	E	22	LEU
5	E	25	ARG
5	E	44	GLU
5	E	63	GLU
5	E	80	LYS
5	E	82	LEU
5	E	94	GLU
5	E	95	MET
5	E	100	ILE
5	E	142	LEU
5	E	144	LEU
5	E	146	GLU
5	E	151	PRO
5	E	161	THR
6	F	31	GLU
6	F	85	ILE
6	F	101	PHE
6	F	125	GLN
6	F	130	LYS
6	F	147	SER
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	93	LYS
7	G	122	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	205	GLN
1	A	206	GLN
1	A	243	ASN

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	289	ASN
1	A	318	ASN
1	A	370	HIS
1	A	410	HIS
2	B	165	HIS
2	B	205	ASN
2	B	231	GLN
2	B	267	GLN
2	B	284	ASN
2	B	323	GLN
3	C	40	ASN
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	197	GLN
4	D	202	HIS
4	D	231	HIS
4	D	242	ASN
5	E	138	GLN
5	E	167	GLN
6	F	28	GLN
6	F	125	GLN
6	F	129	HIS
6	F	137	HIS
7	G	22	ASN
7	G	48	GLN
7	G	56	GLN
7	G	61	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	A	501	8	28,29,29	1.49	5 (17%)	43,45,45	1.79	10 (23%)
9	ADP	B	395	-	28,29,29	1.50	5 (17%)	43,45,45	1.81	9 (20%)

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	-	0/16/32/32	0/3/3/3
9	ADP	B	395	-	-	0/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	395	ADP	C2-N1	3.85	1.40	1.33
9	A	501	ADP	C2-N1	3.62	1.40	1.33
9	B	395	ADP	PB-O1B	3.44	1.61	1.50
9	A	501	ADP	PB-O1B	3.32	1.60	1.50
9	A	501	ADP	C5-N7	-2.89	1.33	1.39
9	B	395	ADP	C5-N7	-2.85	1.33	1.39
9	A	501	ADP	C8-N9	-2.59	1.33	1.37
9	B	395	ADP	C8-N9	-2.32	1.33	1.37
9	A	501	ADP	C4-N9	-2.10	1.33	1.37
9	B	395	ADP	C4-N9	-2.09	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	-5.58	120.13	128.58
9	A	501	ADP	N3-C2-N1	-5.51	120.24	128.58
9	B	395	ADP	C5-C4-N3	-4.60	120.38	126.72
9	B	395	ADP	C2-N3-C4	4.20	122.09	111.83
9	A	501	ADP	C5-C4-N3	-4.20	120.94	126.72
9	A	501	ADP	C2-N3-C4	4.03	121.67	111.83
9	A	501	ADP	N3-C4-N9	3.09	132.42	127.17
9	A	501	ADP	N9-C8-N7	-3.08	109.57	113.94
9	B	395	ADP	C4-C5-N7	-3.03	107.12	110.58
9	B	395	ADP	N3-C4-N9	2.95	132.18	127.17
9	B	395	ADP	N9-C8-N7	-2.84	109.91	113.94
9	A	501	ADP	O3B-PB-O3A	2.84	114.15	104.64
9	B	395	ADP	C5-N7-C8	2.76	107.79	103.45
9	A	501	ADP	C4-N9-C8	2.75	108.63	105.74
9	A	501	ADP	C5-N7-C8	2.64	107.60	103.45
9	A	501	ADP	C4-C5-N7	-2.60	107.61	110.58
9	B	395	ADP	O3B-PB-O3A	2.22	112.06	104.64
9	B	395	ADP	O4'-C1'-N9	2.15	112.23	108.09
9	A	501	ADP	O4'-C1'-C2'	-2.04	102.24	106.62

There are no chirality outliers.

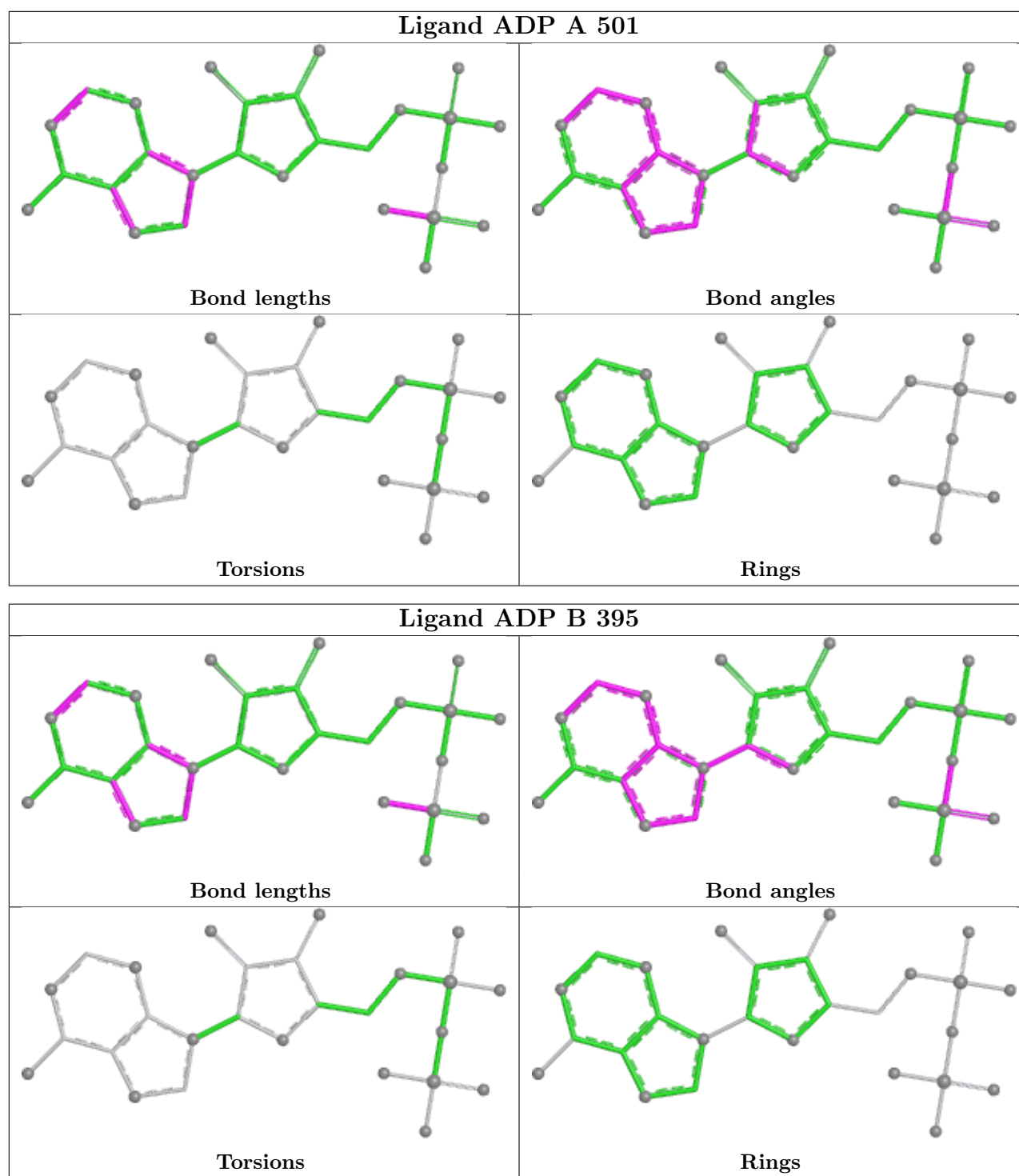
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	501	ADP	3	0
9	B	395	ADP	3	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	388/418 (92%)	0.14	12 (3%) 51 42	30, 56, 84, 103	0
2	B	184/394 (46%)	0.59	25 (13%) 7 5	34, 64, 113, 121	0
3	C	341/372 (91%)	-0.13	5 (1%) 72 64	30, 47, 80, 103	0
4	D	273/300 (91%)	-0.04	2 (0%) 84 79	33, 53, 81, 95	0
5	E	174/178 (97%)	0.49	7 (4%) 42 34	42, 70, 96, 105	0
6	F	165/168 (98%)	-0.03	1 (0%) 85 81	37, 52, 68, 79	0
7	G	128/151 (84%)	0.60	13 (10%) 12 10	42, 80, 106, 118	0
All	All	1653/1981 (83%)	0.16	65 (3%) 43 35	30, 56, 94, 121	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	ALA	5.6
5	E	36	THR	5.4
2	B	187	ARG	4.9
2	B	343	ARG	4.3
2	B	302	VAL	4.0
7	G	40	GLY	3.8
1	A	268	SER	3.7
3	C	319	ALA	3.6
7	G	43	ASP	3.6
5	E	96	TYR	3.6
7	G	9	ALA	3.5
2	B	290	ASP	3.4
1	A	350	SER	3.4
2	B	291	ILE	3.4
2	B	276	VAL	3.3
2	B	337	LEU	3.3
5	E	175	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	334	VAL	3.1
4	D	206	PRO	3.1
5	E	28	PHE	3.0
1	A	80	HIS	2.9
2	B	174	SER	2.9
1	A	249	GLY	2.9
7	G	151	VAL	2.9
7	G	47	ARG	2.9
2	B	342	ILE	2.8
7	G	50	ASN	2.8
1	A	354	SER	2.8
1	A	79	ARG	2.8
5	E	27	GLN	2.7
2	B	336	LYS	2.7
2	B	169	VAL	2.7
2	B	331	LYS	2.6
7	G	118	SER	2.6
2	B	175	LEU	2.5
2	B	176	PRO	2.5
7	G	46	LEU	2.5
6	F	4	THR	2.5
2	B	338	SER	2.4
5	E	86	ASN	2.4
2	B	184	ILE	2.4
1	A	265	LYS	2.4
1	A	359	LYS	2.3
1	A	260	ASN	2.3
7	G	22	ASN	2.3
7	G	18	GLU	2.3
1	A	348	LYS	2.3
3	C	372	VAL	2.3
2	B	274	GLU	2.2
2	B	281	LEU	2.2
3	C	127	GLN	2.2
2	B	154	GLY	2.2
1	A	39	GLU	2.2
7	G	74	ARG	2.2
7	G	26	ASP	2.2
7	G	24	PHE	2.2
3	C	288	PRO	2.2
2	B	162	GLY	2.2
2	B	339	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	340	PHE	2.2
2	B	341	LYS	2.1
4	D	159	ASP	2.1
5	E	29	LYS	2.1
2	B	181	ARG	2.1
3	C	280	SER	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](#)

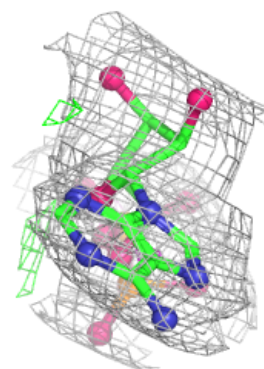
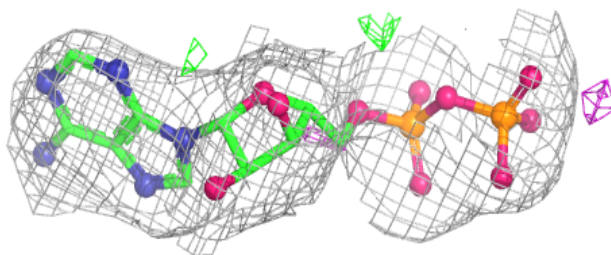
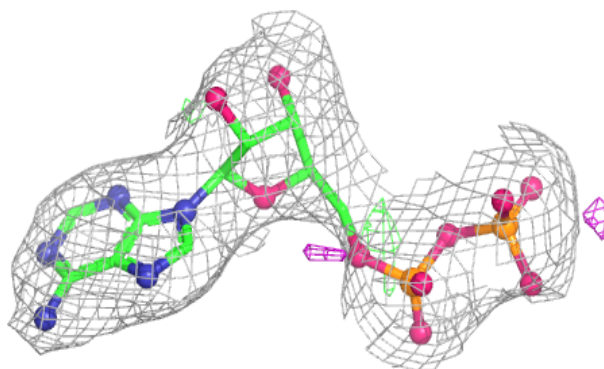
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ADP	B	395	27/27	0.88	0.11	59,64,77,78	0
9	ADP	A	501	27/27	0.93	0.10	50,56,68,70	0
8	CA	A	500	1/1	0.96	0.14	73,73,73,73	0

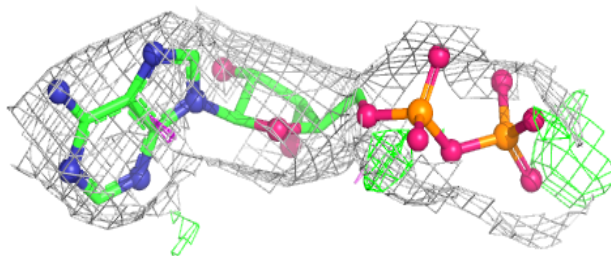
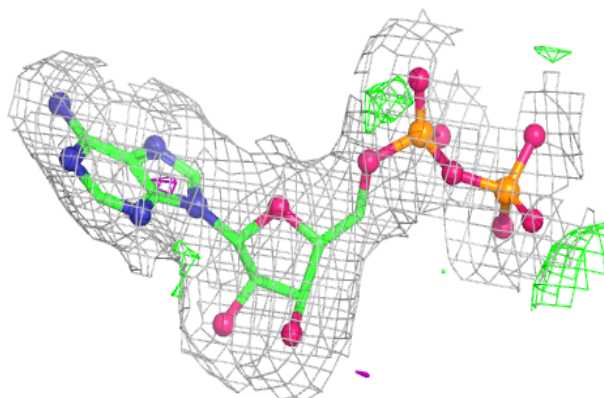
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.