



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:13 AM UTC

PDB ID : 4CJ7 / pdb_00004cj7
Title : Structure of Crenactin, an archeal actin-like protein
Authors : Izore, T.; Duman, R.E.; Kureisaite-Ciziene, D.; Lowe, J.
Deposited on : 2013-12-19
Resolution : 3.20 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

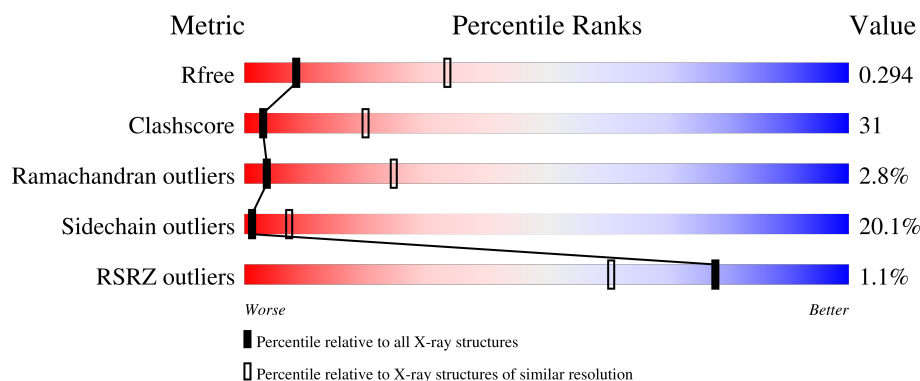
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	432	41% 42% 14% ..
1	B	432	40% 47% 11% ..

2 Entry composition [i](#)

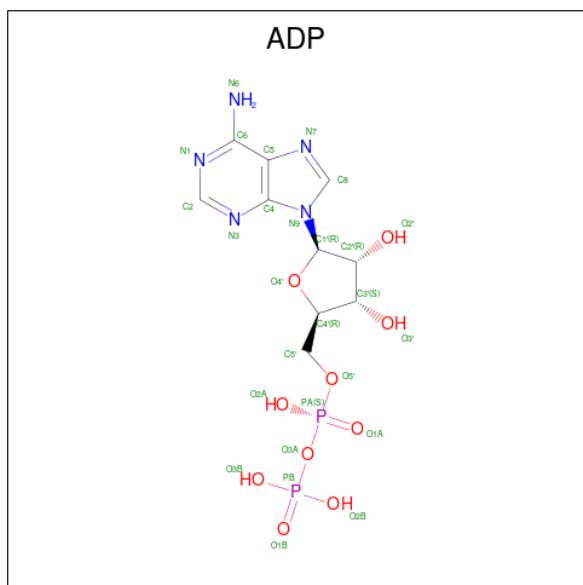
There are 2 unique types of molecules in this entry. The entry contains 6782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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/ACTIN FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3362	2155	576	625	6			
1	B	426	Total	C	N	O	S	0	0	0
			3366	2158	577	625	6			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

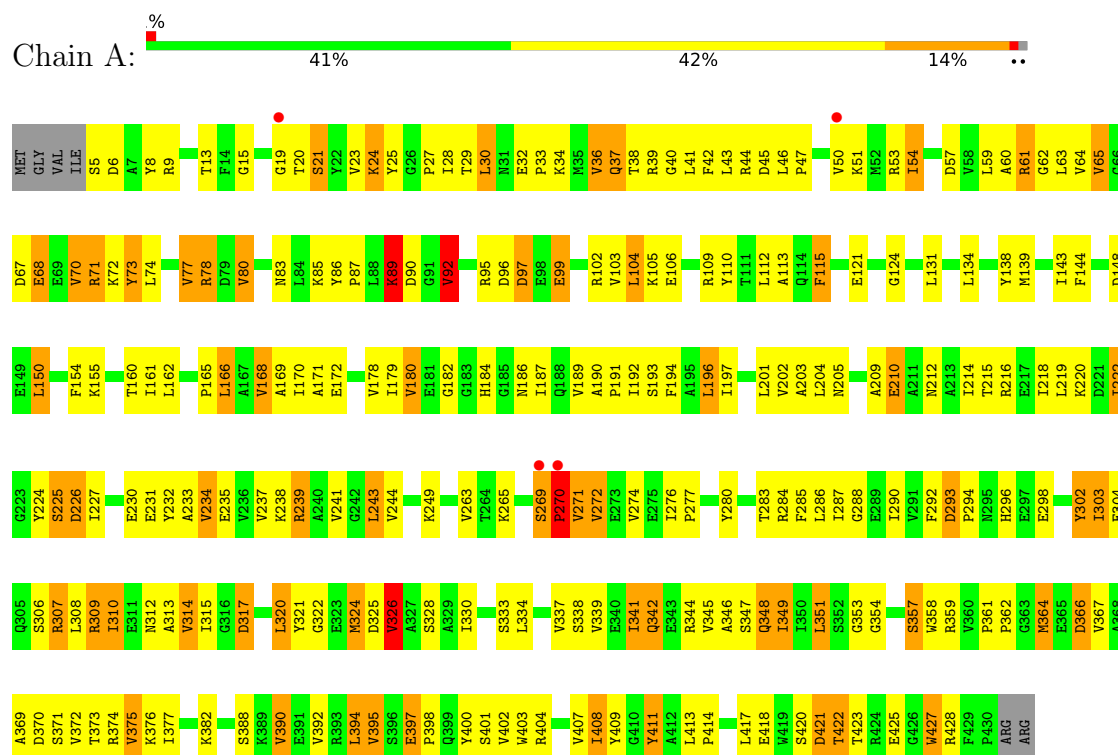


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

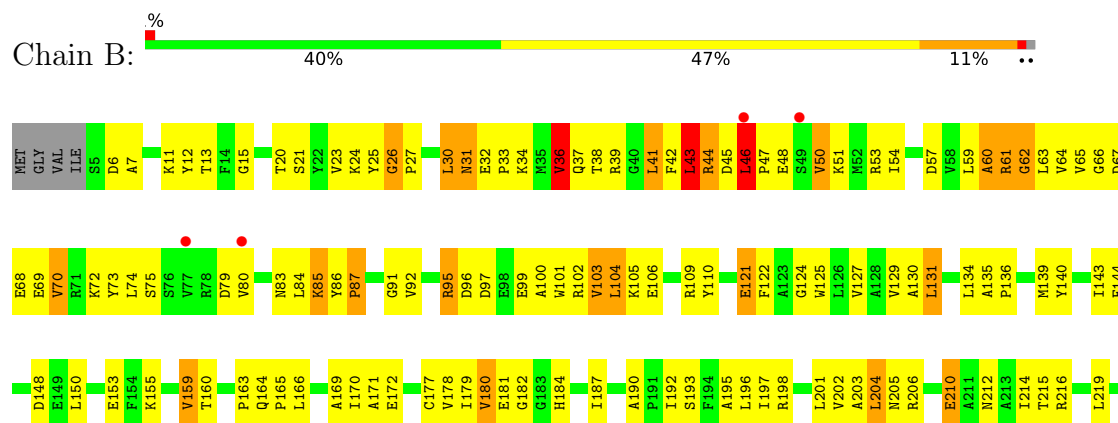
3 Residue-property plots

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/ACTIN FAMILY PROTEIN



• Molecule 1: ACTIN/ACTIN FAMILY PROTEIN



M364	E297	I222	E365	G223	Y224	Y232	A233	A234	E235	V236	V237	K238	L243	V244	P245	R246	R247	L248	K249	E250	A251	I252	R253	K256	K265	V266	R267	L268	S269	P270	V271	V272	E273	V274	E275	I276	P277	R278	E279	Y280	T283	R284	F285	L286	I287	G288	E289	I290	V291	F292	D293	P294	N295	H296
E366	E299	K300	S301	Y302	I303	E304	Q305	S306	R307	L308	R309	I310	E311	N312	A313	V314	I315	G316	D317	L320	Y321	D325	V326	A327	S328	A329	I330	I331	L334	R335	N336	V337	S338	V339	E340	I341	Q342	F343	R344	V345	A346	S347	Q348	I349	I350	L351	S352	G353	G354	S357	P361	P362	G363	
D366	V367	A368	A369	D370	S371	V372	T373	R374	V375	F376	I377	A378	L379	S383	F384	A385	L386	A387	V390	F391	V392	R393	L394	V395	S396	Q399	Y400	S401	V402	W403	R404	V407	I408	Y411	L417	E418	T423	R424	E425	G426	W427	R428	F429	P430	ARG	ARG								

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.13Å 78.13Å 418.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 3.20 48.86 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.86-3.20) 99.9 (48.86-3.20)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.235 , 0.295 0.234 , 0.294	Depositor DCC
R_{free} test set	1129 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6782	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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

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	0.86	5/3432 (0.1%)	1.39	26/4667 (0.6%)
1	B	0.81	1/3436 (0.0%)	1.28	26/4671 (0.6%)
All	All	0.83	6/6868 (0.1%)	1.34	52/9338 (0.6%)

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
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	VAL	CA-C	8.06	1.63	1.52
1	A	272	VAL	CA-CB	7.63	1.63	1.54
1	A	359	ARG	CZ-NH2	-7.29	1.24	1.33
1	A	92	VAL	C-O	6.86	1.31	1.24
1	B	344	ARG	NE-CZ	-6.37	1.26	1.33
1	A	269	SER	C-O	-5.22	1.17	1.24

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	SER	CA-C-N	21.98	147.31	119.84
1	A	269	SER	C-N-CA	21.98	147.31	119.84
1	B	46	LEU	CA-C-N	9.27	129.85	119.93
1	B	46	LEU	C-N-CA	9.27	129.85	119.93
1	A	269	SER	C-N-CD	-8.82	88.82	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	VAL	N-CA-C	-8.72	102.33	111.58
1	B	276	ILE	CA-C-N	8.56	129.08	119.92
1	B	276	ILE	C-N-CA	8.56	129.08	119.92
1	B	6	ASP	N-CA-C	8.34	123.29	112.12
1	A	272	VAL	N-CA-C	8.03	119.84	108.36
1	A	293	ASP	CA-C-N	7.72	129.49	119.84
1	A	293	ASP	C-N-CA	7.72	129.49	119.84
1	A	89	LYS	N-CA-C	-7.66	103.01	111.36
1	A	115	PHE	CA-C-N	-7.39	113.07	120.31
1	A	115	PHE	C-N-CA	-7.39	113.07	120.31
1	A	71	ARG	NE-CZ-NH2	7.16	125.65	119.20
1	B	103	VAL	CB-CA-C	-6.74	103.34	111.97
1	B	292	PHE	N-CA-C	6.59	119.80	111.69
1	B	85	LYS	N-CA-C	6.50	119.00	108.34
1	B	295	ASN	N-CA-C	6.48	118.32	109.11
1	A	6	ASP	N-CA-C	6.39	120.90	112.72
1	A	293	ASP	N-CA-C	6.39	123.94	109.81
1	B	26	GLY	CA-C-N	6.23	126.20	119.78
1	B	26	GLY	C-N-CA	6.23	126.20	119.78
1	B	430	PRO	N-CA-C	6.13	127.42	112.10
1	B	135	ALA	CA-C-N	6.01	126.35	119.92
1	B	135	ALA	C-N-CA	6.01	126.35	119.92
1	B	87	PRO	N-CA-C	-6.00	102.19	111.13
1	A	293	ASP	C-N-CD	-5.92	100.75	125.00
1	A	422	THR	N-CA-C	5.90	120.48	113.28
1	B	95	ARG	N-CA-C	5.90	121.11	111.37
1	A	70	VAL	N-CA-C	-5.81	104.16	112.35
1	B	272	VAL	N-CA-C	5.78	117.07	109.21
1	A	397	GLU	CA-C-N	5.64	125.75	119.32
1	A	397	GLU	C-N-CA	5.64	125.75	119.32
1	A	309	ARG	N-CA-C	5.59	118.07	110.35
1	B	36	VAL	N-CA-C	5.53	115.85	108.27
1	B	7	ALA	N-CA-C	-5.40	105.50	111.71
1	A	210	GLU	N-CA-C	-5.40	105.43	112.23
1	B	336	ASN	N-CA-C	5.39	119.55	112.92
1	A	222	ILE	N-CA-C	-5.36	105.50	110.53
1	B	70	VAL	N-CA-C	-5.32	105.94	111.58
1	A	427	TRP	N-CA-C	5.32	118.60	110.20
1	A	21	SER	N-CA-C	-5.31	105.87	112.93
1	B	43	LEU	N-CA-C	5.30	119.75	113.28
1	B	163	PRO	N-CA-C	5.28	119.51	111.11
1	A	317	ASP	N-CA-C	-5.22	105.77	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	VAL	N-CA-C	5.17	115.36	108.27
1	A	303	ILE	N-CA-C	-5.11	106.94	113.22
1	B	140	TYR	N-CA-C	-5.05	105.48	111.69
1	A	270	PRO	O-C-N	5.04	129.45	122.64
1	B	247	ARG	N-CA-C	-5.02	100.86	109.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	GLY	Peptide

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	3362	0	3398	213	2
1	B	3366	0	3409	225	1
2	A	27	0	12	5	0
2	B	27	0	12	6	0
All	All	6782	0	6831	427	2

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 31.

All (427) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LYS:HD3	1:B:275:GLU:OE1	1.31	1.23
1:A:54:ILE:HD11	1:A:73:TYR:HE2	1.06	1.10
1:A:197:ILE:HG21	1:A:337:VAL:HG12	1.38	1.04
1:B:45:ASP:HB2	1:B:83:ASN:HD21	0.92	1.04
1:B:265:LYS:HG2	1:B:275:GLU:CG	1.87	1.04
1:B:265:LYS:HG2	1:B:275:GLU:CB	1.87	1.03
1:B:265:LYS:CD	1:B:275:GLU:OE1	2.05	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HD11	1:A:73:TYR:CE2	1.93	1.03
1:B:45:ASP:HB2	1:B:83:ASN:ND2	1.74	1.02
1:B:45:ASP:CB	1:B:83:ASN:HD21	1.73	1.01
1:B:265:LYS:HG2	1:B:275:GLU:HG3	1.43	1.00
1:B:265:LYS:CG	1:B:275:GLU:HG3	1.93	0.99
1:B:41:LEU:HD12	1:B:83:ASN:O	1.70	0.91
1:B:134:LEU:HD21	1:B:320:LEU:HD11	1.53	0.90
1:B:180:VAL:HG13	1:B:351:LEU:HD23	1.50	0.90
1:B:54:ILE:HD11	1:B:73:TYR:CE2	2.07	0.90
1:A:134:LEU:HD21	1:A:320:LEU:HD11	1.52	0.89
1:B:20:THR:H	2:B:1431:ADP:PB	1.96	0.89
1:B:197:ILE:HG21	1:B:337:VAL:HG12	1.53	0.88
1:B:265:LYS:CG	1:B:275:GLU:CG	2.51	0.88
1:A:344:ARG:HH12	1:B:72:LYS:HB3	1.40	0.86
1:A:38:THR:HG22	1:A:38:THR:O	1.74	0.85
1:B:178:VAL:CG1	1:B:349:ILE:HD13	2.08	0.83
1:B:178:VAL:HG12	1:B:349:ILE:HD13	1.59	0.83
1:A:312:ASN:OD1	1:A:321:TYR:HA	1.79	0.83
1:B:54:ILE:HD11	1:B:73:TYR:HE2	1.41	0.81
1:B:203:ALA:HB3	1:B:320:LEU:CD1	2.11	0.80
1:B:212:ASN:OD1	1:B:238:LYS:HE2	1.81	0.80
1:A:23:VAL:HG23	1:A:38:THR:OG1	1.78	0.80
1:A:193:SER:HB3	1:B:75:SER:HB2	1.62	0.80
1:B:39:ARG:HB3	1:B:86:TYR:CE1	2.17	0.79
1:A:197:ILE:HG21	1:A:337:VAL:CG1	2.13	0.79
1:A:326:VAL:O	1:A:330:ILE:HG13	1.82	0.78
1:B:265:LYS:HG2	1:B:275:GLU:HB2	1.65	0.78
1:A:409:TYR:CE1	1:A:413:LEU:HD13	2.19	0.78
1:B:47:PRO:HB2	1:B:50:VAL:HG13	1.66	0.78
1:A:361:PRO:HG2	1:A:364:MET:SD	2.24	0.77
1:B:66:GLY:HA3	1:B:69:GLU:OE1	1.83	0.77
1:B:203:ALA:CB	1:B:320:LEU:HD12	2.13	0.77
1:A:172:GLU:OE2	1:A:395:VAL:HG13	1.85	0.77
1:A:186:ASN:HB2	1:A:204:LEU:O	1.86	0.76
1:B:222:ILE:HD13	1:B:277:PRO:HD2	1.67	0.76
1:B:315:ILE:HG12	1:B:320:LEU:HD21	1.67	0.75
1:B:222:ILE:HG12	1:B:280:TYR:HD2	1.51	0.75
1:B:31:ASN:H	1:B:31:ASN:ND2	1.85	0.75
1:A:193:SER:HB3	1:B:75:SER:CB	2.17	0.74
1:A:337:VAL:HG23	1:A:342:GLN:HG2	1.69	0.74
1:B:192:ILE:HD13	1:B:196:LEU:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LYS:HG3	1:B:275:GLU:HG3	1.70	0.73
1:A:302:TYR:O	1:A:306:SER:HB2	1.88	0.73
1:A:166:LEU:O	1:A:166:LEU:HD12	1.89	0.73
1:B:21:SER:N	2:B:1431:ADP:O3B	2.20	0.72
1:A:373:THR:HG22	1:A:377:ILE:HD11	1.73	0.71
1:B:41:LEU:CD1	1:B:83:ASN:O	2.38	0.71
1:B:312:ASN:OD1	1:B:321:TYR:HA	1.90	0.71
1:A:269:SER:O	1:A:272:VAL:N	2.23	0.70
1:A:341:ILE:HD11	1:A:344:ARG:HD2	1.72	0.70
1:A:203:ALA:HB3	1:A:320:LEU:HD12	1.73	0.70
1:B:361:PRO:HG2	1:B:364:MET:SD	2.31	0.70
1:A:203:ALA:CB	1:A:320:LEU:HD12	2.22	0.69
1:B:101:TRP:HH2	1:B:139:MET:HG3	1.57	0.69
1:A:216:ARG:HH12	1:A:307:ARG:HB2	1.57	0.69
1:B:39:ARG:HB3	1:B:86:TYR:CD1	2.28	0.68
1:B:181:GLU:HG3	1:B:352:SER:HB3	1.74	0.68
1:A:95:ARG:HA	1:A:138:TYR:CE1	2.29	0.67
1:A:230:GLU:O	1:A:233:ALA:HB3	1.94	0.67
1:A:21:SER:N	2:A:1431:ADP:O3B	2.27	0.67
1:A:39:ARG:HB3	1:A:86:TYR:CE1	2.30	0.67
1:B:232:TYR:O	1:B:236:VAL:HG23	1.94	0.67
1:B:265:LYS:HD3	1:B:275:GLU:CD	2.19	0.67
1:A:334:LEU:CD1	1:A:346:ALA:HB2	2.24	0.67
1:A:341:ILE:CD1	1:A:344:ARG:HD2	2.26	0.66
1:A:344:ARG:O	1:A:347:SER:HB3	1.96	0.66
1:A:42:PHE:HA	1:A:62:GLY:O	1.95	0.66
1:B:251:ALA:HA	1:B:367:VAL:HG21	1.78	0.66
1:B:44:ARG:HH22	1:B:102:ARG:HH21	1.44	0.66
1:B:203:ALA:HB1	1:B:320:LEU:HD12	1.77	0.66
1:A:72:LYS:C	1:A:73:TYR:HD1	2.03	0.66
1:A:45:ASP:HB3	1:A:78:ARG:HB2	1.79	0.65
1:B:216:ARG:NH1	1:B:307:ARG:HD3	2.12	0.65
1:B:386:LEU:HD12	1:B:390:VAL:HG23	1.78	0.65
1:B:46:LEU:CD2	1:B:50:VAL:HG22	2.27	0.65
1:B:302:TYR:O	1:B:306:SER:HB2	1.96	0.65
1:A:106:GLU:HG2	1:A:109:ARG:HH21	1.61	0.65
1:A:110:TYR:O	1:A:113:ALA:HB3	1.97	0.65
1:A:171:ALA:HA	1:A:408:ILE:HD11	1.79	0.65
1:B:47:PRO:HB2	1:B:50:VAL:CG1	2.25	0.65
1:B:309:ARG:CD	1:B:309:ARG:H	2.10	0.64
1:B:23:VAL:HG23	1:B:38:THR:OG1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ALA:HB3	1:B:320:LEU:HD13	1.78	0.64
1:B:222:ILE:HG12	1:B:280:TYR:CD2	2.31	0.64
1:B:57:ASP:O	1:B:60:ALA:HB3	1.97	0.63
1:A:27:PRO:HD2	1:A:30:LEU:HD21	1.79	0.63
1:A:269:SER:C	1:A:272:VAL:H	2.06	0.63
1:A:193:SER:CB	1:B:75:SER:HB2	2.27	0.63
1:B:105:LYS:HE2	1:B:150:LEU:HD21	1.79	0.62
1:A:36:VAL:HG21	1:A:110:TYR:CE1	2.35	0.62
1:B:346:ALA:O	1:B:390:VAL:HG22	1.99	0.62
1:A:265:LYS:HA	1:A:274:VAL:O	1.98	0.62
1:B:249:LYS:HE2	1:B:296:HIS:HD2	1.65	0.62
1:B:160:THR:HG22	1:B:427:TRP:CZ3	2.35	0.62
1:B:354:GLY:O	1:B:357:SER:HB2	1.98	0.62
1:A:344:ARG:NH1	1:B:72:LYS:HB3	2.11	0.62
1:A:99:GLU:O	1:A:103:VAL:HG23	1.98	0.62
1:A:169:ALA:HB2	1:A:179:ILE:CD1	2.30	0.62
1:B:41:LEU:HB3	1:B:64:VAL:HG12	1.81	0.62
1:A:238:LYS:NZ	2:A:1431:ADP:O2'	2.30	0.62
1:A:61:ARG:C	1:A:63:LEU:H	2.06	0.62
1:B:72:LYS:HZ2	1:B:73:TYR:HE1	1.47	0.62
1:A:89:LYS:HG2	1:A:90:ASP:N	2.15	0.61
1:B:203:ALA:CB	1:B:320:LEU:CD1	2.76	0.61
1:B:92:VAL:HG21	1:B:315:ILE:HG21	1.82	0.61
1:A:216:ARG:HB2	1:A:234:VAL:HG11	1.81	0.61
1:B:72:LYS:NZ	1:B:73:TYR:HE1	1.98	0.61
1:A:184:HIS:CD2	1:A:209:ALA:HB2	2.36	0.60
1:A:194:PHE:HE2	1:B:53:ARG:HD2	1.66	0.60
1:A:216:ARG:NH1	1:A:307:ARG:HD3	2.16	0.60
1:B:31:ASN:H	1:B:31:ASN:HD22	1.48	0.60
1:B:206:ARG:NH2	1:B:291:VAL:O	2.35	0.60
1:A:325:ASP:HB3	1:A:328:SER:H	1.67	0.59
1:A:24:LYS:N	1:A:24:LYS:HD3	2.18	0.59
1:A:170:ILE:HG22	1:A:408:ILE:HG13	1.84	0.59
1:B:180:VAL:CG1	1:B:351:LEU:HD23	2.27	0.59
1:B:129:VAL:HG12	1:B:131:LEU:CD2	2.32	0.59
1:A:227:ILE:HG22	1:A:233:ALA:HB1	1.84	0.59
1:B:206:ARG:HB2	1:B:210:GLU:HG2	1.83	0.59
1:B:334:LEU:O	1:B:337:VAL:HG22	2.03	0.59
1:A:269:SER:C	1:A:271:VAL:H	2.07	0.59
1:B:54:ILE:CD1	1:B:73:TYR:HE2	2.15	0.59
1:B:337:VAL:HG23	1:B:342:GLN:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:HD1	1:A:73:TYR:N	2.01	0.59
1:A:334:LEU:O	1:A:337:VAL:HG22	2.03	0.59
1:B:243:LEU:O	1:B:288:GLY:HA3	2.04	0.58
1:B:127:VAL:HB	1:B:159:VAL:HG13	1.85	0.58
1:A:73:TYR:N	1:A:73:TYR:CD1	2.69	0.58
1:A:341:ILE:HD11	1:A:344:ARG:CD	2.33	0.58
1:B:61:ARG:C	1:B:63:LEU:H	2.11	0.58
1:B:72:LYS:C	1:B:73:TYR:HD1	2.11	0.58
1:B:210:GLU:HB3	1:B:290:ILE:HD13	1.84	0.58
1:A:205:ASN:HB2	1:A:320:LEU:HB2	1.85	0.58
1:A:361:PRO:CG	1:A:364:MET:SD	2.91	0.58
1:A:131:LEU:HD13	1:A:139:MET:HE2	1.86	0.58
1:A:269:SER:O	1:A:271:VAL:N	2.35	0.58
1:B:33:PRO:HD2	1:B:400:TYR:CD1	2.38	0.58
1:B:265:LYS:HG2	1:B:275:GLU:CA	2.34	0.58
1:A:215:THR:OG1	1:A:238:LYS:HB2	2.04	0.57
1:B:105:LYS:HE2	1:B:150:LEU:CD2	2.33	0.57
1:B:344:ARG:HA	1:B:347:SER:HB3	1.86	0.57
1:A:212:ASN:OD1	1:A:238:LYS:HE2	2.04	0.57
1:A:212:ASN:OD1	1:A:238:LYS:CE	2.52	0.57
1:B:383:SER:OG	1:B:385:ALA:HB3	2.04	0.57
1:B:46:LEU:CD2	1:B:50:VAL:CG2	2.82	0.57
1:A:310:ILE:HD12	1:A:310:ILE:O	2.05	0.57
1:B:41:LEU:HD13	1:B:84:LEU:HD13	1.87	0.57
1:A:39:ARG:HB3	1:A:86:TYR:CD1	2.40	0.57
1:A:36:VAL:HG21	1:A:110:TYR:HE1	1.69	0.57
1:A:160:THR:HG22	1:A:427:TRP:CZ3	2.40	0.56
1:B:214:ILE:HG21	1:B:287:ILE:HA	1.87	0.56
1:A:334:LEU:HD11	1:A:346:ALA:HB2	1.87	0.56
1:A:216:ARG:HD2	1:A:307:ARG:NH1	2.20	0.56
1:B:166:LEU:O	1:B:170:ILE:HG13	2.05	0.56
1:A:38:THR:O	1:A:38:THR:CG2	2.49	0.56
1:A:162:LEU:HD23	1:A:162:LEU:H	1.70	0.56
1:A:292:PHE:HZ	1:A:371:SER:HB3	1.70	0.56
1:A:284:ARG:HA	1:A:287:ILE:HD12	1.87	0.56
1:B:373:THR:HG22	1:B:377:ILE:HD11	1.88	0.56
1:B:27:PRO:O	1:B:30:LEU:HG	2.06	0.55
1:B:265:LYS:CG	1:B:275:GLU:HB2	2.35	0.55
1:A:263:VAL:HG13	1:A:276:ILE:O	2.05	0.55
1:B:66:GLY:CA	1:B:69:GLU:OE1	2.53	0.55
1:A:87:PRO:CG	1:A:104:LEU:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD13	1:A:346:ALA:HB2	1.88	0.55
1:B:46:LEU:HB3	1:B:51:LYS:HE2	1.89	0.55
1:B:265:LYS:CG	1:B:275:GLU:CB	2.75	0.55
1:A:184:HIS:ND1	2:A:1431:ADP:O3'	2.32	0.55
1:A:70:VAL:O	1:A:74:LEU:HG	2.07	0.55
1:A:414:PRO:HD2	1:B:48:GLU:HG2	1.89	0.55
1:A:46:LEU:CD2	1:A:50:VAL:HG23	2.36	0.54
1:B:326:VAL:O	1:B:330:ILE:HG13	2.07	0.54
1:A:241:VAL:HG23	1:A:287:ILE:HD13	1.88	0.54
1:A:354:GLY:O	1:A:357:SER:HB2	2.07	0.54
1:B:130:ALA:C	1:B:131:LEU:HD23	2.33	0.54
1:A:68:GLU:O	1:A:71:ARG:HB3	2.08	0.53
1:A:420:SER:O	1:A:422:THR:N	2.40	0.53
1:A:45:ASP:H	1:A:83:ASN:HD21	1.56	0.53
1:A:33:PRO:HG2	1:A:400:TYR:CD1	2.43	0.53
1:A:420:SER:OG	1:A:423:THR:HB	2.08	0.53
1:B:283:THR:HA	1:B:286:LEU:HD13	1.90	0.53
1:A:178:VAL:HG13	1:A:349:ILE:HG23	1.90	0.53
1:A:57:ASP:O	1:A:60:ALA:HB3	2.09	0.53
1:B:179:ILE:HD12	1:B:192:ILE:HG13	1.91	0.53
1:A:394:LEU:HD12	1:A:395:VAL:N	2.24	0.52
1:B:286:LEU:N	1:B:286:LEU:HD12	2.23	0.52
1:A:413:LEU:O	1:A:427:TRP:NE1	2.42	0.52
1:B:212:ASN:O	1:B:215:THR:HB	2.08	0.52
1:A:46:LEU:HD22	1:A:47:PRO:O	2.09	0.52
1:A:249:LYS:HE2	1:A:296:HIS:HD2	1.75	0.52
1:B:106:GLU:HG2	1:B:109:ARG:HH21	1.74	0.52
1:B:87:PRO:HG2	1:B:104:LEU:HD13	1.91	0.52
1:B:129:VAL:HG12	1:B:131:LEU:HD23	1.92	0.52
1:B:178:VAL:HG11	1:B:349:ILE:HD13	1.89	0.52
1:A:269:SER:CB	1:A:270:PRO:HD2	2.36	0.52
1:B:69:GLU:H	1:B:69:GLU:CD	2.18	0.51
1:B:70:VAL:O	1:B:74:LEU:HG	2.09	0.51
1:A:374:ARG:HA	1:A:377:ILE:HD12	1.92	0.51
1:A:227:ILE:CG2	1:A:233:ALA:HB1	2.41	0.51
1:B:205:ASN:HB2	1:B:320:LEU:HB2	1.93	0.51
1:B:386:LEU:HD12	1:B:390:VAL:CG2	2.41	0.51
1:A:328:SER:OG	1:A:382:LYS:HE3	2.11	0.51
1:A:219:LEU:HD11	1:A:237:VAL:HG21	1.93	0.51
1:A:269:SER:HB2	1:A:270:PRO:HD2	1.92	0.51
1:A:124:GLY:HA2	1:A:155:LYS:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:H	1:A:320:LEU:HD22	1.75	0.51
1:B:27:PRO:HD2	1:B:30:LEU:HD21	1.92	0.50
1:A:39:ARG:HA	1:A:85:LYS:O	2.12	0.50
1:A:269:SER:C	1:A:271:VAL:N	2.69	0.50
1:A:313:ALA:HB3	1:A:320:LEU:HD23	1.92	0.50
1:A:411:TYR:CD1	1:A:411:TYR:C	2.88	0.50
1:A:190:ALA:HB2	1:A:201:LEU:HD13	1.92	0.50
1:A:235:GLU:HG3	1:A:239:ARG:HD2	1.93	0.50
1:A:192:ILE:HD13	1:A:196:LEU:HA	1.94	0.50
1:A:314:VAL:C	1:A:315:ILE:HD13	2.36	0.50
1:B:184:HIS:ND1	2:B:1431:ADP:H3'	2.27	0.50
1:A:277:PRO:HD2	1:A:280:TYR:HB2	1.94	0.49
1:B:327:ALA:O	1:B:331:ILE:HG12	2.12	0.49
1:A:244:VAL:HB	1:A:369:ALA:O	2.11	0.49
1:B:43:LEU:N	1:B:62:GLY:O	2.42	0.49
1:B:244:VAL:HB	1:B:369:ALA:O	2.12	0.49
1:B:303:ILE:HD13	1:B:310:ILE:HD11	1.94	0.49
1:A:64:VAL:HG13	1:A:70:VAL:HG22	1.95	0.49
1:B:205:ASN:HB2	1:B:320:LEU:CB	2.42	0.49
1:B:325:ASP:HB3	1:B:328:SER:H	1.77	0.49
1:A:404:ARG:O	1:A:408:ILE:HG12	2.12	0.49
1:B:36:VAL:HG21	1:B:110:TYR:HE2	1.77	0.49
1:A:162:LEU:HD12	1:A:166:LEU:HG	1.93	0.49
1:A:243:LEU:HB3	1:A:285:PHE:CD1	2.48	0.49
1:B:20:THR:HB	2:B:1431:ADP:O3B	2.12	0.49
1:B:245:PRO:CG	1:B:289:GLU:HB2	2.43	0.49
1:B:57:ASP:O	1:B:60:ALA:CB	2.59	0.49
1:B:91:GLY:O	1:B:139:MET:HE1	2.13	0.49
1:B:46:LEU:HA	1:B:47:PRO:HD2	1.65	0.49
1:A:162:LEU:HB3	1:A:409:TYR:CE2	2.48	0.48
1:B:219:LEU:HD11	1:B:237:VAL:HG21	1.95	0.48
1:B:39:ARG:O	1:B:65:VAL:HG22	2.12	0.48
1:B:243:LEU:HB3	1:B:285:PHE:CD1	2.48	0.48
1:A:216:ARG:NH1	1:A:307:ARG:HB2	2.27	0.48
1:A:224:TYR:CE2	1:A:274:VAL:HG13	2.47	0.48
1:B:172:GLU:OE2	1:B:395:VAL:HG13	2.13	0.48
1:B:265:LYS:HA	1:B:275:GLU:HA	1.95	0.48
1:A:373:THR:HG22	1:A:377:ILE:CD1	2.43	0.48
1:B:129:VAL:HG12	1:B:131:LEU:HD21	1.96	0.48
1:B:386:LEU:CD1	1:B:390:VAL:CG2	2.92	0.48
1:B:33:PRO:HG3	1:B:403:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLN:NE2	1:A:39:ARG:HD3	2.28	0.48
1:A:346:ALA:O	1:A:390:VAL:HG22	2.14	0.48
1:A:87:PRO:HG3	1:A:104:LEU:HD13	1.96	0.48
1:A:192:ILE:CD1	1:A:196:LEU:HA	2.44	0.48
1:B:65:VAL:CG1	1:B:66:GLY:N	2.77	0.48
1:A:243:LEU:HD13	1:A:285:PHE:CE1	2.48	0.48
1:A:302:TYR:N	1:A:302:TYR:CD1	2.82	0.48
1:B:42:PHE:CZ	1:B:99:GLU:HB2	2.49	0.48
1:A:243:LEU:CD1	1:A:285:PHE:CE1	2.97	0.48
1:A:193:SER:O	1:A:194:PHE:HB2	2.13	0.47
1:A:197:ILE:HG22	1:A:197:ILE:O	2.14	0.47
1:A:312:ASN:OD1	1:A:322:GLY:N	2.43	0.47
1:A:41:LEU:HD12	1:A:83:ASN:O	2.14	0.47
1:A:203:ALA:O	1:A:320:LEU:HA	2.14	0.47
1:B:224:TYR:CE2	1:B:274:VAL:HG13	2.49	0.47
1:A:144:PHE:CE1	1:A:428:ARG:HB2	2.50	0.47
1:A:367:VAL:HG22	1:A:367:VAL:O	2.14	0.47
1:B:265:LYS:CG	1:B:275:GLU:OE1	2.60	0.47
1:B:364:MET:C	1:B:366:ASP:N	2.72	0.47
1:B:370:ASP:OD2	1:B:372:VAL:HG23	2.15	0.47
1:B:187:ILE:HB	1:B:204:LEU:HD23	1.97	0.47
1:B:423:THR:HG23	1:B:425:GLU:HG2	1.97	0.47
1:A:39:ARG:O	1:A:65:VAL:HG22	2.15	0.47
1:A:61:ARG:C	1:A:63:LEU:N	2.73	0.47
1:A:420:SER:O	1:A:421:ASP:C	2.58	0.47
1:A:214:ILE:HG21	1:A:287:ILE:HA	1.98	0.46
1:A:216:ARG:HH11	1:A:307:ARG:HD3	1.81	0.46
1:A:191:PRO:HG3	1:A:333:SER:OG	2.16	0.46
1:A:9:ARG:NE	1:A:411:TYR:O	2.48	0.46
1:A:62:GLY:H	1:A:102:ARG:HH12	1.63	0.46
1:B:301:SER:O	1:B:304:GLU:HB3	2.16	0.46
1:A:220:LYS:NZ	1:A:307:ARG:HD2	2.30	0.46
1:B:265:LYS:CD	1:B:275:GLU:HB2	2.45	0.46
1:A:77:VAL:HB	1:A:80:VAL:HG22	1.97	0.46
1:A:232:TYR:CD1	1:A:232:TYR:C	2.94	0.46
1:A:348:GLN:HA	1:A:348:GLN:NE2	2.29	0.46
1:B:192:ILE:HD11	1:B:196:LEU:HD12	1.97	0.46
1:A:27:PRO:C	1:A:29:THR:H	2.24	0.46
1:B:265:LYS:HG2	1:B:275:GLU:HA	1.96	0.46
1:A:238:LYS:HD2	1:A:239:ARG:N	2.30	0.46
1:A:414:PRO:CD	1:B:48:GLU:HG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASP:C	1:A:92:VAL:H	2.24	0.46
1:A:269:SER:O	1:A:271:VAL:HB	2.16	0.46
1:B:310:ILE:HD12	1:B:310:ILE:O	2.15	0.46
1:A:283:THR:HA	1:A:286:LEU:HD13	1.98	0.46
1:B:41:LEU:HD12	1:B:41:LEU:HA	1.73	0.46
1:B:184:HIS:ND1	2:B:1431:ADP:C3'	2.79	0.46
1:B:429:PHE:CD1	1:B:429:PHE:N	2.84	0.46
1:B:20:THR:N	2:B:1431:ADP:PB	2.78	0.45
1:B:121:GLU:O	1:B:122:PHE:C	2.58	0.45
1:B:177:CYS:HB3	1:B:348:GLN:HB3	1.98	0.45
1:B:193:SER:C	1:B:195:ALA:H	2.24	0.45
1:A:404:ARG:HA	1:A:407:VAL:HG22	1.99	0.45
1:B:39:ARG:HB3	1:B:86:TYR:HE1	1.78	0.45
1:A:212:ASN:OD1	1:A:238:LYS:HE3	2.16	0.45
1:B:245:PRO:HG3	1:B:289:GLU:HB2	1.99	0.45
1:A:97:ASP:OD1	1:A:97:ASP:C	2.59	0.45
1:B:284:ARG:HA	1:B:287:ILE:HD12	1.99	0.45
1:A:15:GLY:O	1:A:25:TYR:HA	2.16	0.45
1:B:38:THR:HG22	1:B:38:THR:O	2.17	0.45
1:B:292:PHE:HZ	1:B:371:SER:HB3	1.80	0.45
1:A:203:ALA:HB1	1:A:320:LEU:HD12	1.96	0.45
1:A:224:TYR:O	1:A:226:ASP:N	2.50	0.45
1:B:429:PHE:HA	1:B:430:PRO:HD3	1.78	0.45
1:B:87:PRO:HG3	1:B:103:VAL:HB	1.98	0.45
1:A:165:PRO:HA	1:A:168:VAL:HG23	1.98	0.45
1:A:182:GLY:O	1:A:353:GLY:HA3	2.17	0.45
1:A:361:PRO:O	1:A:362:PRO:C	2.59	0.45
1:A:375:VAL:HG11	1:A:392:VAL:HG21	1.99	0.45
1:B:99:GLU:O	1:B:103:VAL:HG23	2.17	0.45
1:B:309:ARG:H	1:B:309:ARG:HD2	1.79	0.45
1:A:20:THR:H	2:A:1431:ADP:PB	2.40	0.45
1:B:180:VAL:CG1	1:B:351:LEU:CD2	2.95	0.45
1:B:289:GLU:OE2	1:B:293:ASP:HB3	2.17	0.45
1:A:178:VAL:CG1	1:A:349:ILE:HD13	2.47	0.44
1:A:238:LYS:HG2	1:A:287:ILE:CG2	2.48	0.44
1:B:235:GLU:OE2	1:B:238:LYS:HE3	2.17	0.44
1:A:397:GLU:N	1:A:398:PRO:CD	2.80	0.44
1:A:187:ILE:HB	1:A:204:LEU:HD23	1.98	0.44
1:B:65:VAL:HG12	1:B:66:GLY:N	2.32	0.44
1:B:109:ARG:NH1	1:B:153:GLU:OE2	2.51	0.44
1:A:33:PRO:HG2	1:A:400:TYR:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:CG2	1:A:287:ILE:HA	2.47	0.44
1:A:341:ILE:CD1	1:A:344:ARG:CD	2.92	0.44
1:B:25:TYR:CZ	1:B:34:LYS:HB2	2.53	0.44
1:B:26:GLY:HA3	1:B:30:LEU:HD11	1.99	0.44
1:B:233:ALA:O	1:B:237:VAL:HG23	2.17	0.44
1:A:397:GLU:N	1:A:398:PRO:HD3	2.33	0.44
1:B:351:LEU:HB2	1:B:394:LEU:HA	2.00	0.44
1:A:232:TYR:CD1	1:A:232:TYR:O	2.71	0.43
1:B:169:ALA:HB2	1:B:179:ILE:HD11	2.00	0.43
1:A:231:GLU:C	1:A:233:ALA:N	2.75	0.43
1:B:171:ALA:HA	1:B:408:ILE:HD11	1.99	0.43
1:B:269:SER:HB2	1:B:270:PRO:HD2	2.00	0.43
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.92	0.43
1:B:41:LEU:HD13	1:B:84:LEU:CD1	2.47	0.43
1:B:373:THR:O	1:B:374:ARG:C	2.57	0.43
1:B:31:ASN:ND2	1:B:31:ASN:N	2.61	0.43
1:B:170:ILE:HG22	1:B:408:ILE:HG13	2.00	0.43
1:B:269:SER:O	1:B:271:VAL:N	2.51	0.43
1:A:40:GLY:HA2	1:A:65:VAL:HG23	2.00	0.43
1:B:386:LEU:O	1:B:387:ALA:C	2.61	0.43
1:B:404:ARG:HA	1:B:407:VAL:HG22	2.00	0.43
1:A:162:LEU:HD22	1:A:409:TYR:HD2	1.83	0.43
1:A:344:ARG:HH12	1:B:72:LYS:CB	2.21	0.43
1:A:351:LEU:O	1:A:395:VAL:HG23	2.18	0.43
1:A:131:LEU:HD11	1:A:143:ILE:HG13	2.01	0.43
1:B:276:ILE:HA	1:B:277:PRO:HD2	1.71	0.43
1:B:165:PRO:O	1:B:179:ILE:HD13	2.19	0.43
1:A:409:TYR:HE1	1:A:413:LEU:HD13	1.76	0.43
1:B:386:LEU:CD1	1:B:390:VAL:HG23	2.48	0.43
1:A:8:TYR:OH	1:A:124:GLY:N	2.52	0.42
1:A:33:PRO:HD2	1:A:400:TYR:CD1	2.54	0.42
1:A:184:HIS:ND1	2:A:1431:ADP:C3'	2.82	0.42
1:A:193:SER:CB	1:B:75:SER:CB	2.89	0.42
1:A:214:ILE:HD12	1:A:214:ILE:HA	1.79	0.42
1:B:164:GLN:N	1:B:165:PRO:CD	2.82	0.42
1:A:46:LEU:HB3	1:A:51:LYS:HE2	2.01	0.42
1:B:11:LYS:HD2	1:B:12:TYR:CE2	2.54	0.42
1:B:39:ARG:HA	1:B:85:LYS:O	2.20	0.42
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.70	0.42
1:A:166:LEU:HD12	1:A:166:LEU:C	2.44	0.42
1:B:15:GLY:O	1:B:25:TYR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ILE:HD13	1:B:277:PRO:CD	2.43	0.42
1:A:61:ARG:O	1:A:63:LEU:N	2.52	0.42
1:B:232:TYR:CD1	1:B:232:TYR:C	2.98	0.42
1:A:27:PRO:C	1:A:29:THR:N	2.76	0.42
1:B:129:VAL:CG1	1:B:131:LEU:HD21	2.50	0.42
1:A:376:LYS:O	1:A:377:ILE:C	2.61	0.42
1:B:190:ALA:HB2	1:B:201:LEU:CD1	2.49	0.42
1:A:191:PRO:O	1:A:192:ILE:HD13	2.20	0.42
1:A:243:LEU:O	1:A:288:GLY:HA3	2.20	0.42
1:B:87:PRO:HB3	1:B:100:ALA:HB1	2.01	0.42
1:A:194:PHE:HD2	1:B:50:VAL:HB	1.85	0.42
1:A:324:MET:O	1:A:325:ASP:HB2	2.19	0.42
1:B:121:GLU:H	1:B:121:GLU:HG2	1.72	0.42
1:B:124:GLY:HA2	1:B:155:LYS:O	2.20	0.42
1:B:182:GLY:O	1:B:353:GLY:HA3	2.19	0.42
1:B:361:PRO:O	1:B:362:PRO:C	2.63	0.41
1:A:222:ILE:HG12	1:A:280:TYR:HD2	1.85	0.41
1:B:243:LEU:HB3	1:B:285:PHE:CE1	2.55	0.41
1:B:21:SER:OG	1:B:184:HIS:HB2	2.20	0.41
1:B:193:SER:HB3	1:B:197:ILE:HD11	2.03	0.41
1:B:379:LEU:O	1:B:383:SER:N	2.54	0.41
1:A:113:ALA:HA	1:A:154:PHE:HE2	1.85	0.41
1:B:320:LEU:N	1:B:320:LEU:HD22	2.36	0.41
1:A:105:LYS:HE3	1:A:150:LEU:HD21	2.02	0.41
1:A:400:TYR:O	1:A:404:ARG:HG3	2.20	0.41
1:B:337:VAL:CG2	1:B:342:GLN:HG2	2.49	0.41
1:B:395:VAL:HG12	1:B:396:SER:O	2.21	0.41
1:A:34:LYS:HG3	1:A:115:PHE:HZ	1.85	0.41
1:A:170:ILE:CG2	1:A:408:ILE:HG13	2.49	0.41
1:A:180:VAL:HA	1:A:189:VAL:HA	2.02	0.41
1:A:216:ARG:HH11	1:A:216:ARG:HG2	1.85	0.41
1:A:358:TRP:CD1	1:A:358:TRP:H	2.37	0.41
1:B:122:PHE:HE2	1:B:155:LYS:HB2	1.85	0.41
1:A:47:PRO:HG2	1:A:50:VAL:CG2	2.50	0.41
1:B:39:ARG:HD3	1:B:86:TYR:HE1	1.85	0.41
1:B:43:LEU:HD12	1:B:43:LEU:HA	1.87	0.40
1:B:54:ILE:CD1	1:B:73:TYR:CE2	2.92	0.40
1:B:72:LYS:HG3	1:B:73:TYR:CE1	2.56	0.40
1:B:134:LEU:O	1:B:136:PRO:HD3	2.21	0.40
1:B:210:GLU:CB	1:B:290:ILE:HD13	2.48	0.40
1:B:227:ILE:HG22	1:B:233:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ILE:H	1:B:310:ILE:HG13	1.77	0.40
1:A:215:THR:HG22	1:A:234:VAL:HG12	2.03	0.40
1:A:220:LYS:HG2	1:A:225:SER:HB3	2.03	0.40
1:A:222:ILE:HD13	1:A:277:PRO:HD3	2.03	0.40
1:B:131:LEU:C	1:B:164:GLN:HG3	2.46	0.40
1:A:42:PHE:HD1	1:A:62:GLY:O	2.04	0.40
1:B:73:TYR:N	1:B:73:TYR:CD1	2.88	0.40
1:B:361:PRO:CG	1:B:364:MET:SD	3.06	0.40
1:B:12:TYR:HA	1:B:125:TRP:CZ3	2.56	0.40
1:B:401:SER:C	1:B:403:TRP:N	2.79	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:SER:OG	1:B:342:GLN:OE1[3_445]	1.67	0.53
1:A:304:GLU:OE2	1:A:304:GLU:OE2[7_645]	1.74	0.46

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	424/432 (98%)	358 (84%)	51 (12%)	15 (4%)	3	20
1	B	424/432 (98%)	356 (84%)	59 (14%)	9 (2%)	5	31
All	All	848/864 (98%)	714 (84%)	110 (13%)	24 (3%)	4	25

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PRO
1	A	294	PRO

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Mol	Chain	Res	Type
1	A	307	ARG
1	A	324	MET
1	A	388	SER
1	A	421	ASP
1	B	307	ARG
1	B	402	VAL
1	A	293	ASP
1	A	366	ASP
1	A	97	ASP
1	B	97	ASP
1	A	239	ARG
1	A	342	GLN
1	B	60	ALA
1	B	62	GLY
1	B	304	GLU
1	A	403	TRP
1	A	411	TYR
1	B	387	ALA
1	B	411	TYR
1	B	270	PRO
1	A	161	ILE
1	A	28	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	357/363 (98%)	284 (80%)	73 (20%)	1	7
1	B	358/363 (99%)	287 (80%)	71 (20%)	1	8
All	All	715/726 (98%)	571 (80%)	144 (20%)	1	7

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER

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Mol	Chain	Res	Type
1	A	13	THR
1	A	24	LYS
1	A	30	LEU
1	A	32	GLU
1	A	36	VAL
1	A	37	GLN
1	A	43	LEU
1	A	44	ARG
1	A	53	ARG
1	A	54	ILE
1	A	59	LEU
1	A	61	ARG
1	A	65	VAL
1	A	67	ASP
1	A	68	GLU
1	A	73	TYR
1	A	77	VAL
1	A	78	ARG
1	A	80	VAL
1	A	89	LYS
1	A	92	VAL
1	A	96	ASP
1	A	99	GLU
1	A	104	LEU
1	A	112	LEU
1	A	121	GLU
1	A	148	ASP
1	A	150	LEU
1	A	166	LEU
1	A	168	VAL
1	A	180	VAL
1	A	196	LEU
1	A	202	VAL
1	A	210	GLU
1	A	218	ILE
1	A	225	SER
1	A	226	ASP
1	A	234	VAL
1	A	243	LEU
1	A	290	ILE
1	A	298	GLU
1	A	302	TYR

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Mol	Chain	Res	Type
1	A	303	ILE
1	A	308	LEU
1	A	309	ARG
1	A	310	ILE
1	A	314	VAL
1	A	317	ASP
1	A	320	LEU
1	A	326	VAL
1	A	338	SER
1	A	339	VAL
1	A	341	ILE
1	A	345	VAL
1	A	348	GLN
1	A	349	ILE
1	A	351	LEU
1	A	357	SER
1	A	364	MET
1	A	366	ASP
1	A	370	ASP
1	A	372	VAL
1	A	375	VAL
1	A	390	VAL
1	A	394	LEU
1	A	395	VAL
1	A	401	SER
1	A	402	VAL
1	A	408	ILE
1	A	417	LEU
1	A	418	GLU
1	A	425	GLU
1	B	13	THR
1	B	24	LYS
1	B	30	LEU
1	B	31	ASN
1	B	32	GLU
1	B	36	VAL
1	B	37	GLN
1	B	41	LEU
1	B	43	LEU
1	B	44	ARG
1	B	46	LEU
1	B	50	VAL

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Mol	Chain	Res	Type
1	B	59	LEU
1	B	61	ARG
1	B	67	ASP
1	B	68	GLU
1	B	79	ASP
1	B	80	VAL
1	B	95	ARG
1	B	96	ASP
1	B	104	LEU
1	B	121	GLU
1	B	131	LEU
1	B	143	ILE
1	B	144	PHE
1	B	148	ASP
1	B	159	VAL
1	B	180	VAL
1	B	198	ARG
1	B	202	VAL
1	B	204	LEU
1	B	210	GLU
1	B	225	SER
1	B	226	ASP
1	B	234	VAL
1	B	238	LYS
1	B	248	LEU
1	B	253	ARG
1	B	256	LYS
1	B	267	ARG
1	B	272	VAL
1	B	278	ARG
1	B	290	ILE
1	B	298	GLU
1	B	300	LYS
1	B	303	ILE
1	B	309	ARG
1	B	310	ILE
1	B	314	VAL
1	B	317	ASP
1	B	320	LEU
1	B	326	VAL
1	B	339	VAL
1	B	341	ILE

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Mol	Chain	Res	Type
1	B	347	SER
1	B	348	GLN
1	B	349	ILE
1	B	357	SER
1	B	366	ASP
1	B	373	THR
1	B	375	VAL
1	B	386	LEU
1	B	392	VAL
1	B	399	GLN
1	B	402	VAL
1	B	404	ARG
1	B	408	ILE
1	B	417	LEU
1	B	418	GLU
1	B	423	THR
1	B	429	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	83	ASN
1	A	296	HIS
1	A	336	ASN
1	A	348	GLN
1	B	31	ASN
1	B	37	GLN
1	B	83	ASN
1	B	176	ASN
1	B	296	HIS
1	B	336	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	ADP	A	1431	-	28,29,29	1.76	5 (17%)	43,45,45	2.20	14 (32%)
2	ADP	B	1431	-	28,29,29	1.65	4 (14%)	43,45,45	2.33	14 (32%)

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
2	ADP	A	1431	-	-	2/16/32/32	0/3/3/3
2	ADP	B	1431	-	-	2/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1431	ADP	C5-C4	5.71	1.49	1.39
2	B	1431	ADP	C5-C4	5.17	1.48	1.39
2	B	1431	ADP	C5-C6	4.11	1.52	1.41
2	A	1431	ADP	C5-C6	3.81	1.51	1.41
2	A	1431	ADP	PA-O3A	3.11	1.62	1.59
2	B	1431	ADP	C8-N7	3.01	1.37	1.31
2	A	1431	ADP	C8-N7	3.00	1.37	1.31
2	B	1431	ADP	C8-N9	-2.22	1.33	1.37
2	A	1431	ADP	C4-N3	2.01	1.38	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1431	ADP	C5-C4-N3	-6.95	117.15	126.72
2	B	1431	ADP	C5-C4-N3	-5.64	118.95	126.72
2	A	1431	ADP	N3-C4-N9	5.32	136.21	127.17
2	B	1431	ADP	C4-C5-N7	-4.89	105.00	110.58
2	B	1431	ADP	C2-N3-C4	4.52	122.86	111.83
2	B	1431	ADP	O4'-C1'-N9	4.37	116.48	108.09
2	A	1431	ADP	C4-C5-N7	-4.33	105.63	110.58
2	B	1431	ADP	C6-C5-N7	4.24	140.27	132.09
2	B	1431	ADP	N3-C2-N1	-4.22	122.19	128.58
2	B	1431	ADP	N3-C4-N9	4.16	134.25	127.17
2	A	1431	ADP	C2-N3-C4	4.02	121.66	111.83
2	A	1431	ADP	O3'-C3'-C2'	-3.90	99.32	111.82
2	B	1431	ADP	C4-N9-C8	3.54	109.45	105.74
2	A	1431	ADP	C5-N7-C8	3.48	108.92	103.45
2	B	1431	ADP	C5-N7-C8	2.89	107.99	103.45
2	A	1431	ADP	O2'-C2'-C3'	-2.89	102.56	111.82
2	B	1431	ADP	C4'-O4'-C1'	-2.78	103.32	109.47
2	B	1431	ADP	O3'-C3'-C2'	-2.73	103.05	111.82
2	A	1431	ADP	C2'-C1'-N9	2.72	120.06	113.30
2	A	1431	ADP	N3-C2-N1	-2.65	124.57	128.58
2	A	1431	ADP	C6-C5-N7	2.52	136.94	132.09
2	A	1431	ADP	O4'-C1'-C2'	-2.49	101.29	106.62
2	A	1431	ADP	C4-N9-C8	2.39	108.24	105.74
2	A	1431	ADP	N9-C8-N7	-2.38	110.56	113.94
2	A	1431	ADP	C4'-O4'-C1'	-2.28	104.42	109.47
2	B	1431	ADP	N9-C8-N7	-2.26	110.73	113.94
2	B	1431	ADP	C4-N9-C1'	-2.15	121.60	126.63
2	B	1431	ADP	O2'-C2'-C3'	-2.03	105.32	111.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

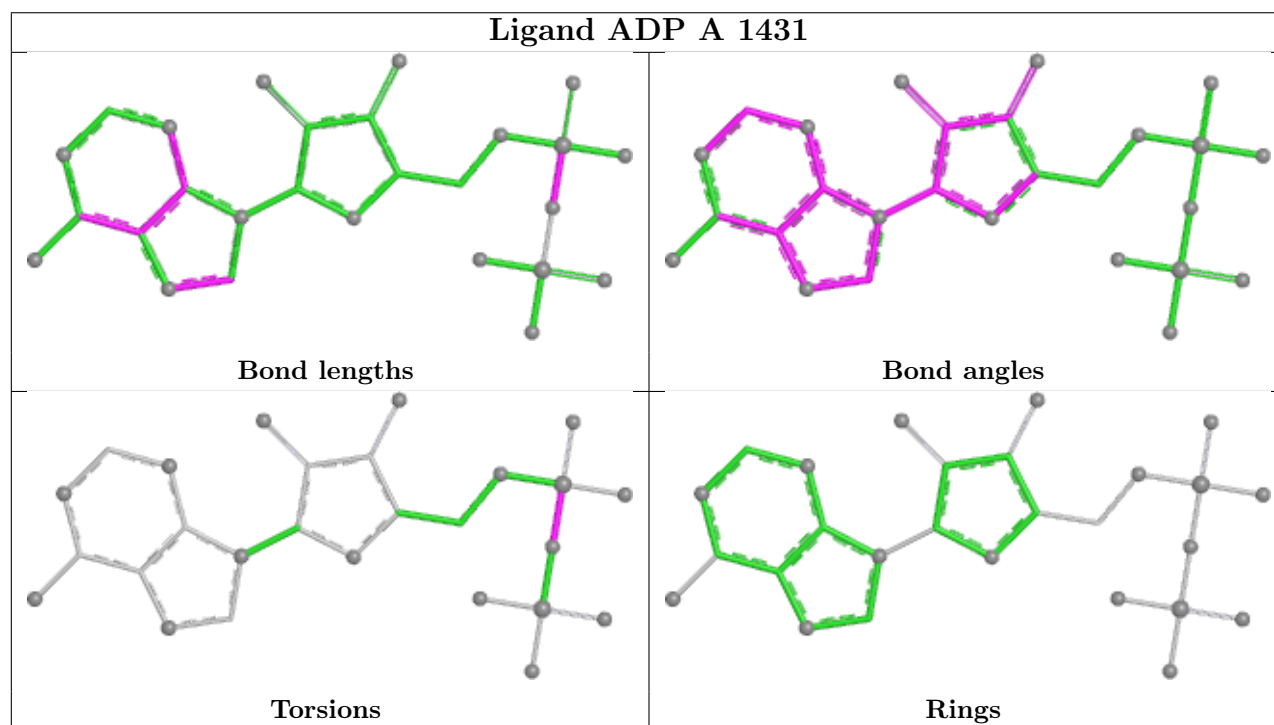
Mol	Chain	Res	Type	Atoms
2	A	1431	ADP	PB-O3A-PA-O1A
2	A	1431	ADP	PB-O3A-PA-O2A
2	B	1431	ADP	PB-O3A-PA-O2A
2	B	1431	ADP	PB-O3A-PA-O1A

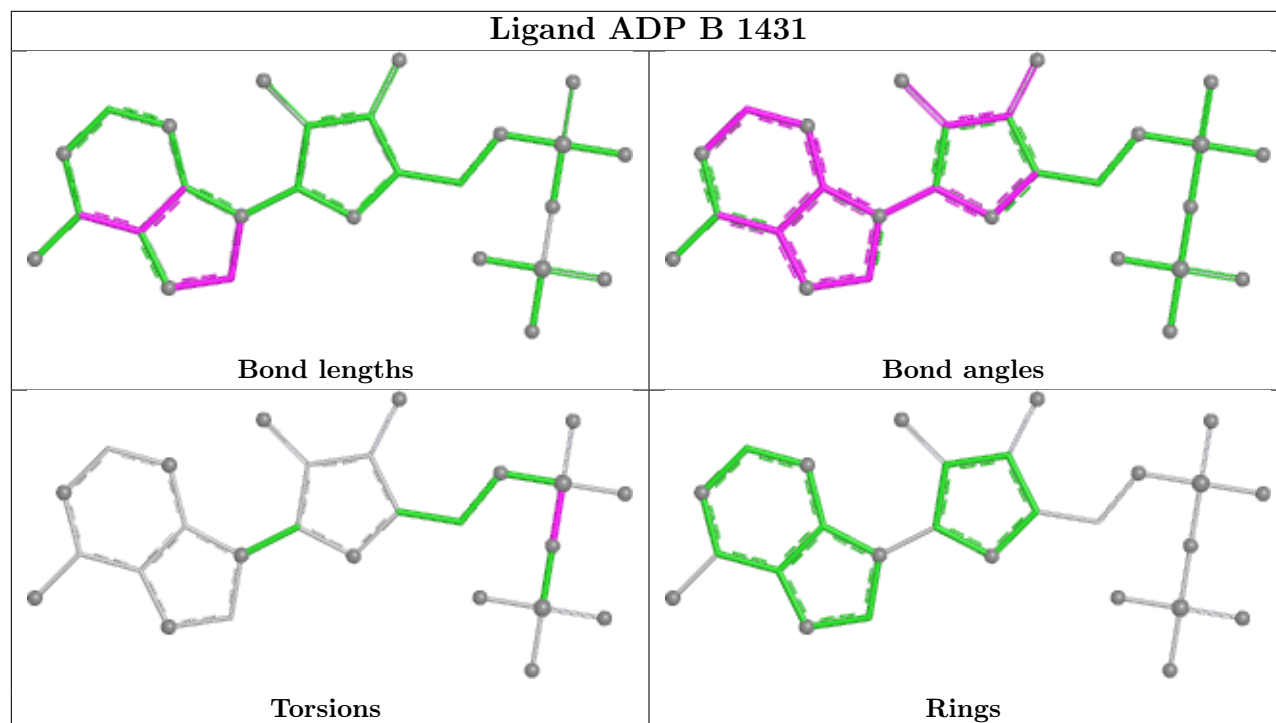
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1431	ADP	5	0
2	B	1431	ADP	6	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	426/432 (98%)	-0.26	4 (0%)	81 64	48, 86, 133, 189	0
1	B	426/432 (98%)	-0.22	5 (1%)	76 58	47, 89, 136, 194	0
All	All	852/864 (98%)	-0.24	9 (1%)	78 61	47, 88, 135, 194	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	VAL	2.9
1	A	270	PRO	2.8
1	A	269	SER	2.4
1	B	46	LEU	2.4
1	B	77	VAL	2.4
1	B	80	VAL	2.4
1	A	19	GLY	2.3
1	B	308	LEU	2.2
1	B	49	SER	2.2

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,

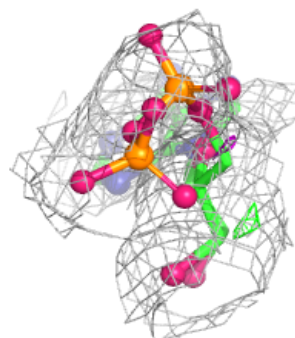
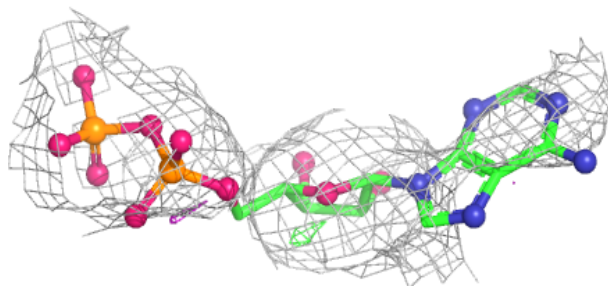
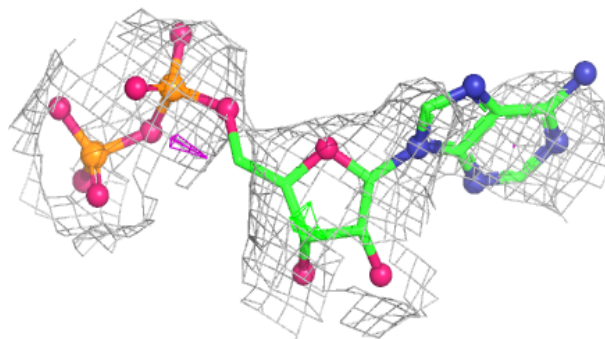
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	1431	27/27	0.87	0.12	94,139,168,173	0
2	ADP	B	1431	27/27	0.87	0.12	90,139,152,156	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.

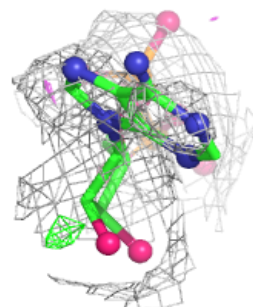
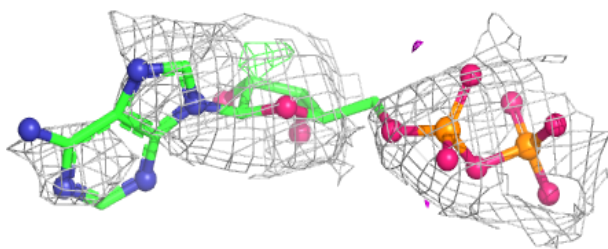
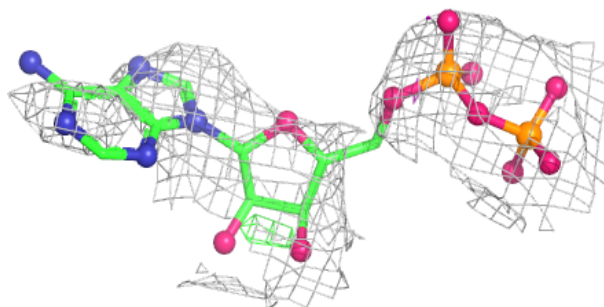
Electron density around ADP A 1431:

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 1431:

$2mF_o - DF_c$ (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.