



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:38 AM UTC

PDB ID : 4PL3 / pdb_00004pl3
Title : Crystal structure of murine IRE1 in complex with MKC9989 inhibitor
Authors : Sanches, M.; Duffy, N.; Talukdar, M.; Thevakumaran, N.; Chiovitti, D.; Al-
awar, R.; Patterson, J.B.; Sicheri, F.
Deposited on : 2014-05-16
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

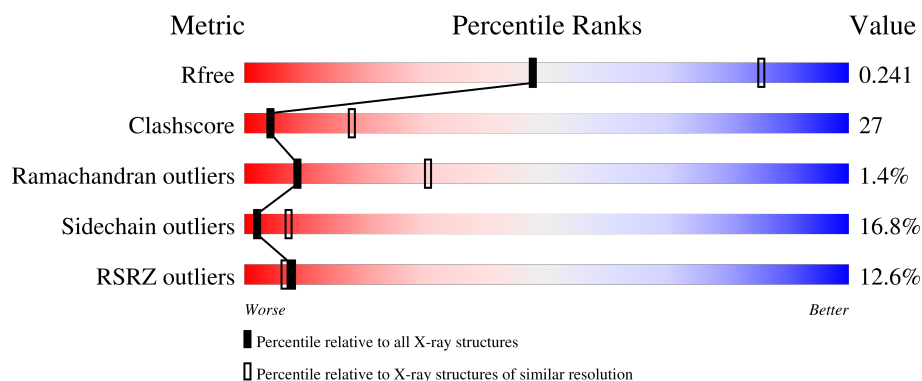
1 Overall quality at a glance

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	435	11% 43% 37% 9% 11%
1	B	435	11% 42% 37% 10% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12482 atoms, of which 6152 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.

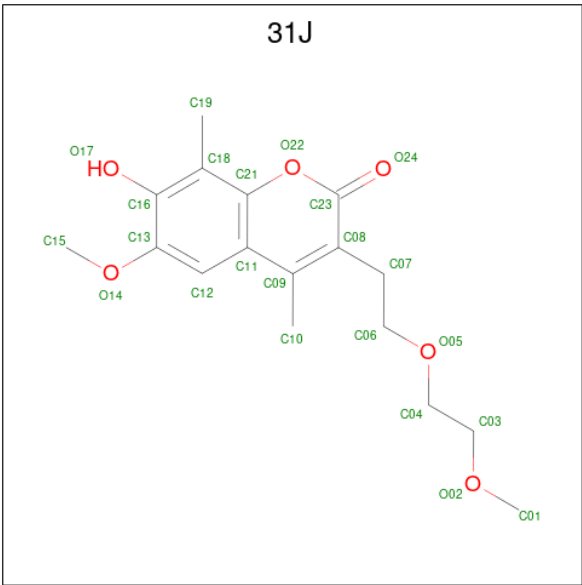
- Molecule 1 is a protein called Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0	0
			6201	2003	3072	541	566	19			
1	B	383	Total	C	H	N	O	S	0	0	0
			6155	1984	3056	541	555	19			

There are 16 discrepancies between the modelled and reference sequences:

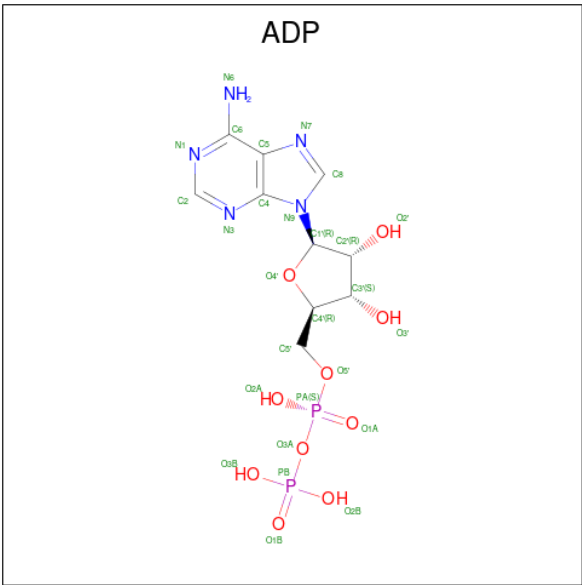
Chain	Residue	Modelled	Actual	Comment	Reference
A	543	GLY	-	expression tag	UNP Q9EQY0
A	544	ALA	-	expression tag	UNP Q9EQY0
A	545	MET	-	expression tag	UNP Q9EQY0
A	546	ASP	-	expression tag	UNP Q9EQY0
A	547	PRO	-	expression tag	UNP Q9EQY0
A	548	GLU	-	expression tag	UNP Q9EQY0
A	549	PHE	-	expression tag	UNP Q9EQY0
A	772	TYR	ASN	engineered mutation	UNP Q9EQY0
B	543	GLY	-	expression tag	UNP Q9EQY0
B	544	ALA	-	expression tag	UNP Q9EQY0
B	545	MET	-	expression tag	UNP Q9EQY0
B	546	ASP	-	expression tag	UNP Q9EQY0
B	547	PRO	-	expression tag	UNP Q9EQY0
B	548	GLU	-	expression tag	UNP Q9EQY0
B	549	PHE	-	expression tag	UNP Q9EQY0
B	772	TYR	ASN	engineered mutation	UNP Q9EQY0

- Molecule 2 is 7-hydroxy-6-methoxy-3-[2-(2-methoxyethoxy)ethyl]-4,8-dimethyl-2H-chromen-2-one (CCD ID: 31J) (formula: C₁₇H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	17	6		
2	B	1	Total	C	O	0	0
			23	17	6		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
3	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

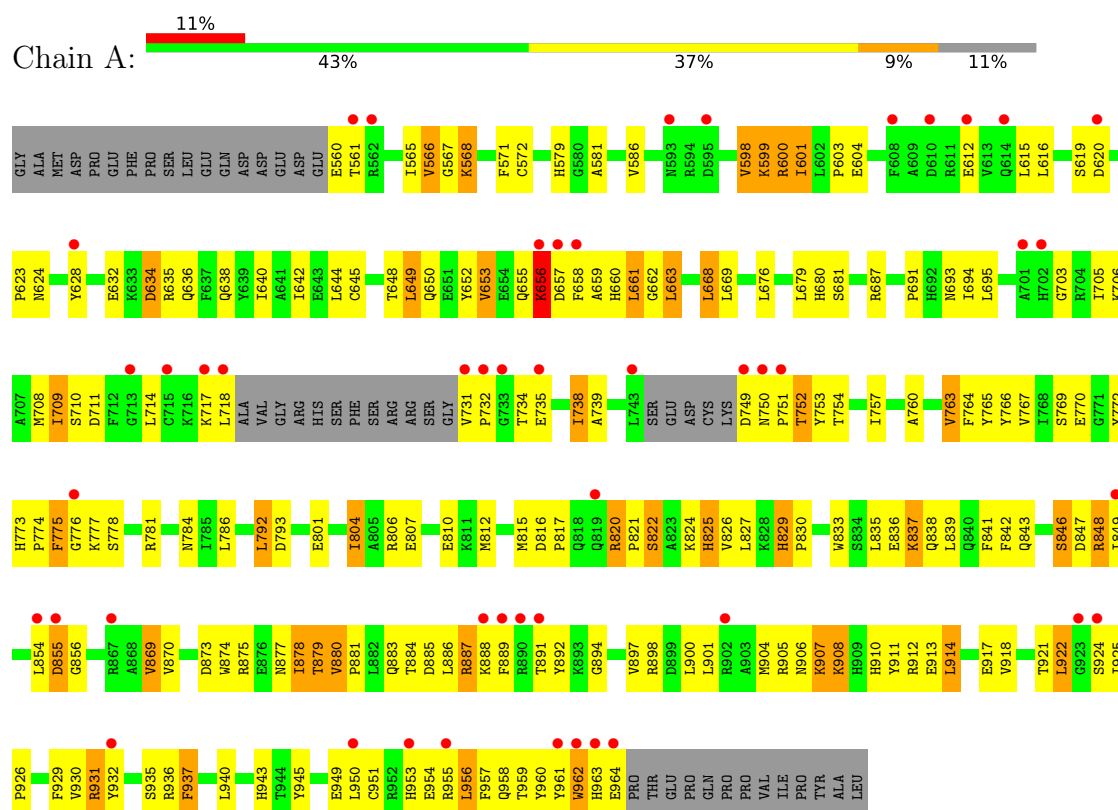
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0

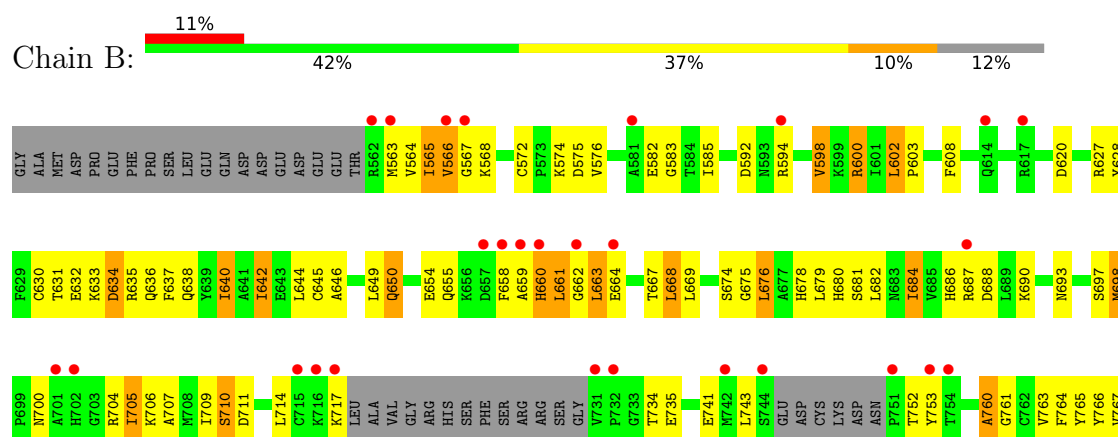
3 Residue-property plots

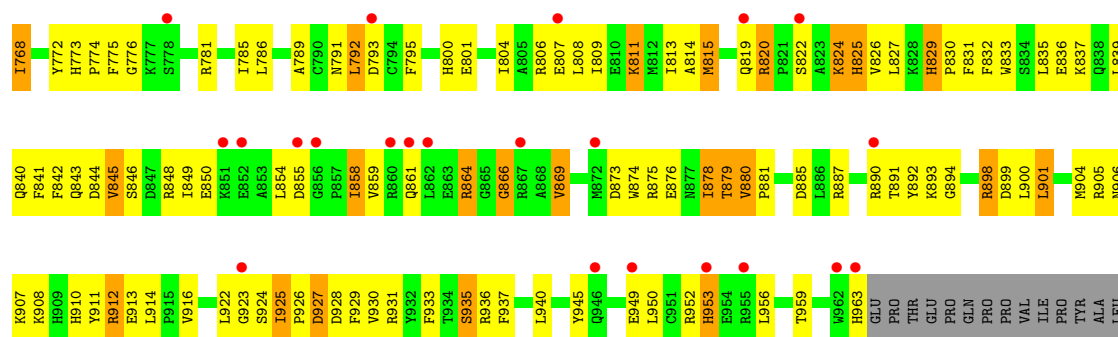
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine/threonine-protein kinase/endoribonuclease IRE1



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.08Å 90.50Å 72.13Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	72.09 – 2.90 72.09 – 2.90	Depositor EDS
% Data completeness (in resolution range)	61.9 (72.09-2.90) 62.0 (72.09-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1175)	Depositor
R, R_{free}	0.201 , 0.234 0.205 , 0.241	Depositor DCC
R_{free} test set	458 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12482	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: MG, ADP, 31J

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	0.72	0/3206	0.99	12/4336 (0.3%)
1	B	0.65	0/3177	0.98	11/4294 (0.3%)
All	All	0.68	0/6383	0.99	23/8630 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	CYS	CA-C-N	7.65	127.32	119.82
1	A	572	CYS	C-N-CA	7.65	127.32	119.82
1	B	831	PHE	N-CA-C	-5.95	104.92	111.82
1	B	660	HIS	N-CA-C	5.87	120.29	113.18
1	A	653	VAL	CB-CA-C	-5.83	104.39	112.02
1	B	710	SER	N-CA-C	5.74	115.68	108.45
1	B	829	HIS	CA-C-N	5.68	126.94	119.84
1	B	829	HIS	C-N-CA	5.68	126.94	119.84
1	A	937	PHE	CA-C-N	5.48	125.57	119.32
1	A	937	PHE	C-N-CA	5.48	125.57	119.32
1	A	835	LEU	N-CA-C	-5.46	105.33	111.28
1	B	768	ILE	CB-CA-C	-5.42	104.75	112.22
1	A	804	ILE	CB-CA-C	-5.34	103.88	112.16
1	A	775	PHE	N-CA-C	5.23	122.15	113.89
1	A	829	HIS	CA-C-N	5.21	126.35	119.84
1	A	829	HIS	C-N-CA	5.21	126.35	119.84
1	B	760	ALA	N-CA-C	-5.21	105.25	111.03
1	A	869	VAL	CB-CA-C	-5.18	105.08	112.22
1	B	688	ASP	N-CA-C	5.09	116.88	108.49
1	A	601	ILE	N-CA-C	5.07	115.61	108.36
1	B	664	GLU	CA-C-N	5.06	124.84	119.28
1	B	664	GLU	C-N-CA	5.06	124.84	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	667	THR	N-CA-C	-5.02	105.99	111.82

There are no chirality outliers.

There are no planarity outliers.

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	3129	3072	3054	163	0
1	B	3099	3056	3038	169	2
2	A	23	0	20	6	2
2	B	23	0	19	0	0
3	A	27	12	12	5	0
3	B	27	12	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	6330	6152	6155	337	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 27.

All (337) 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:843:GLN:OE1	1:B:908:LYS:NZ	1.98	0.97
1:A:910:HIS:CE1	2:A:1001:31J:H14	2.04	0.91
1:A:892:TYR:OH	2:A:1001:31J:O17	1.98	0.82
1:A:932:TYR:O	1:A:936:ARG:NH1	2.15	0.80
1:A:829:HIS:CG	1:A:830:PRO:HD2	2.17	0.80
1:A:855:ASP:OD1	1:A:855:ASP:C	2.25	0.80
1:A:910:HIS:CE1	2:A:1001:31J:C10	2.65	0.79
1:A:603:PRO:O	1:A:717:LYS:NZ	2.16	0.79
1:B:634:ASP:OD1	1:B:635:ARG:N	2.16	0.78
1:B:661:LEU:N	1:B:662:GLY:HA3	1.99	0.78
1:A:836:GLU:HG3	1:A:926:PRO:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ILE:HD13	1:A:821:PRO:O	1.86	0.75
1:A:962:TRP:CD1	1:A:962:TRP:O	2.41	0.73
3:A:1002:ADP:O2B	3:A:1002:ADP:H5'2	1.88	0.73
1:B:904:MET:HG2	1:B:933:PHE:CZ	2.26	0.71
1:B:923:GLY:O	1:B:928:ASP:HB3	1.91	0.71
1:A:880:VAL:O	1:A:884:THR:HG23	1.90	0.71
1:A:849:ILE:HG21	1:A:898:ARG:HD3	1.73	0.70
1:B:924:SER:O	1:B:925:ILE:HB	1.92	0.70
1:B:660:HIS:N	1:B:661:LEU:HA	2.07	0.70
1:A:634:ASP:C	1:A:634:ASP:OD1	2.35	0.70
1:A:949:GLU:O	1:A:950:LEU:HB2	1.91	0.69
1:B:840:GLN:O	1:B:844:ASP:HB2	1.93	0.69
1:B:923:GLY:O	1:B:928:ASP:CB	2.40	0.69
1:B:678:HIS:O	1:B:681:SER:OG	2.08	0.68
1:B:791:ASN:ND2	1:B:793:ASP:OD2	2.27	0.68
1:A:849:ILE:CG2	1:A:898:ARG:HD3	2.23	0.68
1:B:565:ILE:C	1:B:566:VAL:HG23	2.18	0.67
1:A:586:VAL:HG22	1:A:599:LYS:HB2	1.76	0.67
1:B:924:SER:O	1:B:925:ILE:CB	2.43	0.66
1:A:880:VAL:HG23	1:A:881:PRO:HD3	1.77	0.65
1:B:792:LEU:CD2	1:B:792:LEU:N	2.59	0.65
1:A:924:SER:OG	1:A:925:ILE:N	2.28	0.65
1:A:663:LEU:HD12	1:A:663:LEU:O	1.97	0.64
1:B:634:ASP:OD1	1:B:634:ASP:C	2.41	0.64
1:B:676:LEU:HD22	1:B:680:HIS:CE1	2.33	0.64
1:B:628:TYR:CD1	1:B:642:ILE:HG22	2.32	0.64
1:B:661:LEU:HD12	1:B:662:GLY:HA3	1.80	0.64
1:A:773:HIS:CD2	1:A:774:PRO:HD2	2.33	0.64
1:A:886:LEU:HD22	1:A:892:TYR:CE2	2.32	0.64
1:A:676:LEU:HD11	1:A:680:HIS:NE2	2.12	0.63
1:B:710:SER:OG	1:B:711:ASP:N	2.32	0.63
1:B:892:TYR:OH	1:B:906:ASN:ND2	2.30	0.63
1:B:765:TYR:CE2	1:B:792:LEU:HA	2.33	0.63
1:A:855:ASP:OD1	1:A:856:GLY:N	2.32	0.62
1:B:773:HIS:ND1	1:B:774:PRO:HD2	2.13	0.62
1:A:951:CYS:HB3	1:A:954:GLU:HG3	1.82	0.62
1:B:565:ILE:O	1:B:566:VAL:HG23	1.98	0.62
1:A:806:ARG:HG2	1:A:810:GLU:OE2	2.00	0.62
1:B:598:VAL:HA	1:B:640:ILE:O	1.99	0.62
1:A:668:LEU:HD12	1:A:668:LEU:C	2.25	0.62
1:A:949:GLU:C	1:A:951:CYS:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:HIS:NE2	1:A:962:TRP:CD1	2.69	0.61
1:A:854:LEU:HD12	1:A:855:ASP:N	2.15	0.61
1:B:873:ASP:OD2	1:B:875:ARG:NH1	2.34	0.60
1:A:906:ASN:O	1:A:908:LYS:N	2.33	0.60
1:A:829:HIS:CD2	1:A:830:PRO:HD2	2.36	0.60
1:A:906:ASN:C	1:A:908:LYS:N	2.59	0.60
1:B:800:HIS:O	1:B:804:ILE:HG12	2.02	0.60
1:A:904:MET:HE1	1:A:940:LEU:HD21	1.84	0.60
3:B:1002:ADP:H5'2	3:B:1002:ADP:O1B	2.01	0.59
1:B:814:ALA:O	1:B:820:ARG:NH1	2.35	0.59
1:A:848:ARG:NH1	1:A:954:GLU:OE1	2.34	0.59
1:A:891:THR:O	1:A:891:THR:HG22	2.02	0.59
1:B:668:LEU:C	1:B:668:LEU:HD12	2.27	0.59
1:B:845:VAL:HG12	1:B:846:SER:N	2.18	0.59
1:B:830:PRO:HG3	1:B:945:TYR:CE2	2.38	0.58
1:B:931:ARG:O	1:B:935:SER:HB3	2.03	0.58
1:A:854:LEU:HD12	1:A:854:LEU:C	2.28	0.58
1:A:634:ASP:OD1	1:A:635:ARG:N	2.37	0.57
1:A:792:LEU:N	1:A:792:LEU:CD2	2.68	0.57
1:B:849:ILE:HG13	1:B:850:GLU:N	2.19	0.57
1:B:923:GLY:C	1:B:928:ASP:HB2	2.29	0.57
1:A:822:SER:O	1:A:826:VAL:HG23	2.05	0.57
1:B:600:ARG:HG2	1:B:600:ARG:HH11	1.69	0.57
1:A:849:ILE:HG21	1:A:898:ARG:CD	2.33	0.57
1:A:908:LYS:O	1:A:911:TYR:HB2	2.05	0.57
1:A:870:VAL:HG13	1:A:874:TRP:HB3	1.87	0.57
1:A:910:HIS:O	1:A:914:LEU:HD23	2.04	0.57
1:B:880:VAL:HG13	1:B:881:PRO:HD3	1.87	0.56
1:A:873:ASP:HA	1:A:894:GLY:O	2.05	0.56
1:A:628:TYR:CD1	1:A:642:ILE:HG22	2.40	0.56
1:A:773:HIS:CD2	1:A:774:PRO:CD	2.88	0.56
1:B:908:LYS:HB2	1:B:929:PHE:CZ	2.40	0.56
1:B:764:PHE:O	1:B:768:ILE:HG12	2.05	0.56
1:B:795:PHE:CD2	1:B:806:ARG:HB2	2.40	0.56
1:B:912:ARG:NH2	1:B:913:GLU:OE1	2.39	0.56
1:A:849:ILE:CG2	1:A:898:ARG:CD	2.83	0.56
1:A:906:ASN:O	1:A:907:LYS:C	2.46	0.56
1:A:661:LEU:HD21	1:A:703:GLY:O	2.06	0.55
1:A:765:TYR:CE2	1:A:792:LEU:HA	2.40	0.55
1:B:760:ALA:O	1:B:763:VAL:CG2	2.54	0.55
1:B:824:LYS:HA	1:B:827:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:SER:HB3	1:B:825:HIS:HB2	1.88	0.55
1:A:917:GLU:CD	1:A:917:GLU:H	2.14	0.55
1:B:904:MET:HE1	1:B:940:LEU:HD21	1.89	0.55
1:B:873:ASP:HA	1:B:894:GLY:O	2.06	0.55
1:B:775:PHE:H	1:B:776:GLY:HA2	1.72	0.55
1:A:885:ASP:OD2	1:A:907:LYS:HE3	2.06	0.54
1:B:760:ALA:O	1:B:763:VAL:HG22	2.07	0.54
1:B:660:HIS:N	1:B:661:LEU:CA	2.69	0.54
1:B:792:LEU:N	1:B:792:LEU:HD23	2.22	0.54
1:A:680:HIS:CE1	1:A:753:TYR:HB2	2.42	0.54
1:B:628:TYR:CD1	1:B:642:ILE:CG2	2.91	0.54
1:A:648:THR:O	1:A:649:LEU:C	2.51	0.54
1:B:850:GLU:OE2	1:B:898:ARG:NH1	2.40	0.54
1:B:661:LEU:H	1:B:662:GLY:HA3	1.72	0.53
1:B:830:PRO:HG3	1:B:945:TYR:CD2	2.43	0.53
1:A:962:TRP:CD1	1:A:962:TRP:C	2.86	0.53
1:B:675:GLY:O	1:B:678:HIS:HB3	2.09	0.53
1:B:890:ARG:CB	1:B:892:TYR:HB2	2.39	0.53
1:A:600:ARG:HG2	1:A:600:ARG:HH11	1.74	0.53
1:B:668:LEU:C	1:B:668:LEU:CD1	2.82	0.53
1:A:669:LEU:HD21	1:A:764:PHE:HA	1.90	0.52
1:B:706:LYS:HG2	1:B:707:ALA:N	2.23	0.52
1:A:773:HIS:CE1	1:A:781:ARG:HD3	2.44	0.52
1:B:686:HIS:O	1:B:687:ARG:HB2	2.09	0.52
1:B:822:SER:O	1:B:826:VAL:HG23	2.09	0.51
1:A:953:HIS:C	1:A:955:ARG:H	2.19	0.51
1:B:846:SER:HA	1:B:849:ILE:HG12	1.93	0.51
1:A:874:TRP:CD1	1:A:900:LEU:HB2	2.45	0.51
1:A:877:ASN:O	1:A:936:ARG:HD3	2.11	0.51
1:B:700:ASN:ND2	1:B:704:ARG:HG2	2.26	0.51
1:A:824:LYS:HA	1:A:827:LEU:HD12	1.92	0.51
1:B:927:ASP:HB3	1:B:931:ARG:NH1	2.26	0.51
3:B:1002:ADP:O1B	3:B:1002:ADP:O2A	2.29	0.51
1:B:937:PHE:HB3	1:B:940:LEU:HB2	1.91	0.50
1:B:676:LEU:CD2	1:B:680:HIS:NE2	2.75	0.50
1:B:741:GLU:OE1	1:B:820:ARG:NH2	2.44	0.50
1:B:839:LEU:HD13	1:B:930:VAL:HB	1.94	0.50
1:B:841:PHE:O	1:B:842:PHE:C	2.54	0.50
1:B:874:TRP:O	1:B:878:ILE:HG23	2.11	0.50
1:A:963:HIS:O	1:A:964:GLU:HB2	2.11	0.50
1:B:565:ILE:C	1:B:566:VAL:CG2	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:ASN:C	1:A:908:LYS:H	2.20	0.50
1:A:693:ASN:ND2	1:A:711:ASP:OD2	2.45	0.50
1:B:655:GLN:HB3	1:B:658:PHE:HB2	1.93	0.49
1:A:668:LEU:C	1:A:668:LEU:CD1	2.85	0.49
1:A:922:LEU:HD13	1:A:929:PHE:CE1	2.47	0.49
1:B:661:LEU:HB2	1:B:662:GLY:CA	2.41	0.49
1:A:565:ILE:C	1:A:566:VAL:HG23	2.36	0.49
1:B:874:TRP:HB2	1:B:937:PHE:CZ	2.47	0.49
1:A:579:HIS:O	3:A:1002:ADP:H5'1	2.12	0.49
1:B:891:THR:O	1:B:892:TYR:CD1	2.65	0.49
1:A:812:MET:O	1:A:820:ARG:HG3	2.13	0.49
1:B:661:LEU:N	1:B:662:GLY:CA	2.74	0.49
1:A:738:ILE:O	1:A:739:ALA:C	2.56	0.49
1:A:874:TRP:O	1:A:878:ILE:HG23	2.12	0.49
1:A:879:THR:HG21	1:A:921:THR:HG21	1.94	0.49
1:B:910:HIS:O	1:B:911:TYR:C	2.55	0.49
1:A:642:ILE:CD1	3:A:1002:ADP:N6	2.76	0.48
1:A:833:TRP:CG	1:A:837:LYS:HG2	2.48	0.48
1:B:861:GLN:OE1	1:B:950:LEU:HD11	2.13	0.48
1:B:603:PRO:O	1:B:717:LYS:NZ	2.25	0.48
1:B:697:SER:O	1:B:705:ILE:HD12	2.14	0.48
1:B:923:GLY:O	1:B:928:ASP:HB2	2.10	0.48
1:A:734:THR:O	1:A:735:GLU:C	2.55	0.48
1:B:836:GLU:HG3	1:B:926:PRO:HG2	1.95	0.48
1:B:815:MET:HE2	1:B:815:MET:HA	1.95	0.48
1:B:669:LEU:HD22	1:B:764:PHE:CD1	2.48	0.48
1:B:760:ALA:O	1:B:761:GLY:C	2.56	0.48
1:A:875:ARG:HA	1:A:878:ILE:HD13	1.96	0.48
1:B:705:ILE:CG2	1:B:706:LYS:N	2.75	0.48
1:B:659:ALA:C	1:B:661:LEU:HA	2.39	0.48
1:B:663:LEU:HD22	1:B:705:ILE:HG22	1.95	0.48
1:B:822:SER:O	1:B:825:HIS:HB3	2.14	0.48
1:A:567:GLY:HA2	1:A:568:LYS:C	2.39	0.47
1:B:661:LEU:HD12	1:B:662:GLY:CA	2.43	0.47
1:A:775:PHE:H	1:A:776:GLY:HA2	1.79	0.47
3:A:1002:ADP:H5'2	3:A:1002:ADP:PB	2.53	0.47
1:B:924:SER:O	1:B:925:ILE:HG13	2.13	0.47
1:A:914:LEU:HD12	1:A:918:VAL:CG1	2.45	0.47
1:B:646:ALA:HB2	1:B:698:MET:HG3	1.97	0.47
1:A:652:TYR:CZ	1:A:660:HIS:ND1	2.83	0.47
1:B:608:PHE:CE2	1:B:640:ILE:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:VAL:O	1:B:848:ARG:N	2.42	0.47
1:A:843:GLN:O	1:A:846:SER:N	2.48	0.47
1:A:870:VAL:HG12	1:A:870:VAL:O	2.15	0.47
1:A:900:LEU:HD21	1:A:937:PHE:CE2	2.50	0.47
1:A:931:ARG:O	1:A:935:SER:HB3	2.14	0.47
1:A:841:PHE:O	1:A:842:PHE:C	2.57	0.47
1:B:674:SER:HA	1:B:827:LEU:HD11	1.95	0.47
1:B:801:GLU:CD	1:B:801:GLU:H	2.23	0.47
1:A:841:PHE:HB2	1:A:960:TYR:CE1	2.50	0.47
1:B:900:LEU:HD21	1:B:937:PHE:CD2	2.50	0.47
1:B:904:MET:HG2	1:B:933:PHE:CE1	2.50	0.47
1:A:717:LYS:O	1:A:718:LEU:HG	2.15	0.46
1:A:887:ARG:HD2	1:A:887:ARG:HA	1.58	0.46
1:A:943:HIS:O	1:A:943:HIS:CD2	2.68	0.46
1:B:890:ARG:CB	1:B:892:TYR:N	2.77	0.46
1:B:858:ILE:HD13	1:B:859:VAL:HG23	1.97	0.46
1:A:847:ASP:OD1	1:A:905:ARG:NE	2.49	0.46
1:A:648:THR:HG22	1:A:695:LEU:HD23	1.96	0.46
1:A:777:LYS:O	1:A:778:SER:C	2.58	0.46
1:A:932:TYR:C	1:A:936:ARG:NH1	2.74	0.46
1:B:830:PRO:CG	1:B:945:TYR:CE2	2.99	0.46
1:B:923:GLY:HA2	1:B:924:SER:C	2.40	0.46
1:B:811:LYS:HB2	1:B:811:LYS:NZ	2.29	0.46
1:A:612:GLU:O	1:A:615:LEU:HB3	2.16	0.46
1:A:687:ARG:HD3	1:A:751:PRO:HG3	1.97	0.46
1:B:682:LEU:HB2	1:B:684:ILE:CG2	2.46	0.46
1:A:565:ILE:HG22	1:A:567:GLY:N	2.31	0.46
1:A:957:PHE:C	1:A:959:THR:H	2.24	0.46
1:B:676:LEU:CD2	1:B:680:HIS:CE1	2.99	0.46
1:B:684:ILE:O	1:B:684:ILE:HG12	2.16	0.46
1:B:858:ILE:N	1:B:858:ILE:HD12	2.31	0.46
1:B:880:VAL:HG22	1:B:881:PRO:N	2.31	0.46
1:B:904:MET:HG2	1:B:933:PHE:CE2	2.51	0.46
1:B:866:GLY:O	1:B:869:VAL:HG12	2.17	0.45
1:A:825:HIS:HE2	1:A:962:TRP:CD1	2.34	0.45
1:B:572:CYS:HB3	1:B:575:ASP:OD2	2.17	0.45
1:B:791:ASN:H	1:B:792:LEU:HD23	1.81	0.45
1:B:874:TRP:HB2	1:B:937:PHE:HZ	1.81	0.45
1:A:900:LEU:HD12	1:A:900:LEU:O	2.17	0.45
1:B:567:GLY:O	1:B:632:GLU:OE1	2.34	0.45
1:A:658:PHE:O	1:A:658:PHE:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:HIS:NE2	2:A:1001:31J:C10	2.80	0.45
1:B:565:ILE:O	1:B:566:VAL:CB	2.61	0.45
1:B:761:GLY:HA3	1:B:813:ILE:HG22	1.99	0.45
1:B:829:HIS:CG	1:B:830:PRO:HD2	2.51	0.45
1:A:655:GLN:HB3	1:A:658:PHE:HB2	1.98	0.45
1:A:910:HIS:NE2	2:A:1001:31J:H12	2.32	0.45
1:A:600:ARG:HH11	1:A:600:ARG:CG	2.30	0.45
1:A:804:ILE:O	1:A:804:ILE:HG22	2.16	0.45
1:A:937:PHE:HB3	1:A:940:LEU:HB2	1.99	0.45
1:B:679:LEU:O	1:B:684:ILE:HG23	2.17	0.45
1:B:826:VAL:HG12	1:B:826:VAL:O	2.16	0.45
1:A:760:ALA:O	1:A:763:VAL:HG23	2.17	0.45
1:B:775:PHE:N	1:B:776:GLY:CA	2.80	0.45
1:B:565:ILE:O	1:B:566:VAL:CG2	2.65	0.44
1:B:775:PHE:CD1	1:B:789:ALA:O	2.70	0.44
1:B:680:HIS:CE1	1:B:753:TYR:HB2	2.53	0.44
1:A:567:GLY:O	1:A:632:GLU:OE1	2.36	0.44
1:A:749:ASP:OD1	1:A:750:ASN:N	2.50	0.44
1:A:775:PHE:N	1:A:776:GLY:HA2	2.33	0.44
1:A:792:LEU:N	1:A:792:LEU:HD23	2.33	0.44
1:A:956:LEU:HD12	1:A:956:LEU:O	2.18	0.44
1:B:658:PHE:O	1:B:659:ALA:HB3	2.17	0.44
1:A:624:ASN:O	1:A:708:MET:HA	2.18	0.44
1:A:628:TYR:HA	1:A:642:ILE:HG22	2.00	0.44
1:B:766:TYR:HA	1:B:772:TYR:O	2.18	0.44
1:B:910:HIS:O	1:B:912:ARG:N	2.51	0.44
1:A:693:ASN:ND2	3:A:1002:ADP:O3B	2.51	0.43
1:A:839:LEU:HD13	1:A:930:VAL:HB	2.00	0.43
1:A:649:LEU:O	1:A:650:GLN:C	2.59	0.43
1:A:644:LEU:HD12	1:A:645:CYS:N	2.33	0.43
1:B:574:LYS:O	1:B:576:VAL:N	2.51	0.43
1:B:661:LEU:CB	1:B:662:GLY:CA	2.95	0.43
1:B:815:MET:HE2	1:B:815:MET:CA	2.48	0.43
1:B:879:THR:HG23	1:B:881:PRO:HD2	2.00	0.43
1:A:717:LYS:C	1:A:718:LEU:HG	2.44	0.43
1:B:675:GLY:O	1:B:676:LEU:C	2.61	0.43
1:B:773:HIS:ND1	1:B:774:PRO:CD	2.82	0.43
1:B:912:ARG:CZ	1:B:913:GLU:OE1	2.66	0.43
1:B:953:HIS:HA	1:B:963:HIS:NE2	2.33	0.43
1:A:752:THR:O	1:A:754:THR:N	2.52	0.43
1:A:849:ILE:HG22	1:A:898:ARG:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:924:SER:O	1:B:925:ILE:CG1	2.66	0.43
1:A:619:SER:O	1:A:620:ASP:C	2.61	0.43
1:A:691:PRO:HG3	1:A:766:TYR:CE2	2.54	0.43
1:B:890:ARG:HA	1:B:891:THR:C	2.43	0.43
1:B:949:GLU:O	1:B:952:ARG:N	2.51	0.43
1:A:601:ILE:O	1:A:601:ILE:HG13	2.17	0.43
1:A:824:LYS:O	1:A:827:LEU:HB2	2.19	0.43
1:A:870:VAL:CG1	1:A:874:TRP:HD1	2.32	0.43
1:A:658:PHE:O	1:A:659:ALA:HB3	2.19	0.42
1:A:679:LEU:HD12	1:A:709:ILE:HD11	2.00	0.42
1:B:700:ASN:CG	1:B:704:ARG:HG2	2.44	0.42
1:A:843:GLN:OE1	1:A:908:LYS:NZ	2.51	0.42
1:A:883:GLN:O	1:A:887:ARG:HB2	2.19	0.42
1:A:754:THR:HB	1:A:820:ARG:NH1	2.35	0.42
1:A:960:TYR:HB2	1:A:961:TYR:CD1	2.54	0.42
2:A:1001:31J:H12	2:A:1001:31J:H11	1.87	0.42
1:B:833:TRP:CH2	1:B:945:TYR:HE2	2.37	0.42
1:B:874:TRP:NE1	1:B:894:GLY:HA2	2.34	0.42
1:A:655:GLN:O	1:A:657:ASP:N	2.52	0.42
1:A:829:HIS:CG	1:A:830:PRO:CD	2.96	0.42
1:B:602:LEU:HD13	1:B:637:PHE:CE1	2.55	0.42
1:B:743:LEU:HD22	1:B:786:LEU:HD21	2.02	0.42
1:B:791:ASN:C	1:B:792:LEU:HD23	2.45	0.42
1:B:600:ARG:HH11	1:B:600:ARG:CG	2.33	0.42
1:B:775:PHE:N	1:B:776:GLY:HA2	2.33	0.42
1:B:826:VAL:O	1:B:832:PHE:HE2	2.02	0.42
1:B:885:ASP:OD1	1:B:907:LYS:HE3	2.20	0.42
1:B:924:SER:N	1:B:928:ASP:HB2	2.34	0.42
1:A:869:VAL:HG21	1:A:943:HIS:ND1	2.35	0.42
1:A:652:TYR:CE1	1:A:660:HIS:ND1	2.87	0.42
1:A:801:GLU:CD	1:A:801:GLU:H	2.28	0.42
1:A:932:TYR:CE2	1:A:936:ARG:NH2	2.87	0.42
1:B:760:ALA:HA	1:B:763:VAL:HG22	2.02	0.42
1:B:801:GLU:CD	1:B:801:GLU:N	2.77	0.42
1:B:910:HIS:O	1:B:914:LEU:HD13	2.19	0.42
1:B:890:ARG:HA	1:B:891:THR:OG1	2.19	0.41
1:A:599:LYS:NZ	1:A:714:LEU:HD22	2.36	0.41
1:A:649:LEU:HD13	1:A:653:VAL:HG23	2.03	0.41
1:A:825:HIS:CE1	1:A:962:TRP:NE1	2.88	0.41
1:B:781:ARG:O	1:B:785:ILE:HG13	2.20	0.41
1:A:623:PRO:O	1:A:706:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:ASP:OD1	1:A:816:ASP:C	2.62	0.41
1:A:838:GLN:O	1:A:841:PHE:HB3	2.20	0.41
1:A:571:PHE:CD1	1:A:598:VAL:HG21	2.54	0.41
1:A:905:ARG:O	1:A:905:ARG:CG	2.62	0.41
1:A:887:ARG:C	1:A:889:PHE:H	2.29	0.41
1:B:628:TYR:HD1	1:B:642:ILE:HG22	1.82	0.41
1:A:957:PHE:O	1:A:959:THR:N	2.54	0.41
1:B:693:ASN:ND2	1:B:711:ASP:HB2	2.36	0.41
1:A:655:GLN:O	1:A:656:LYS:C	2.63	0.41
1:B:563:MET:HG3	1:B:564:VAL:N	2.36	0.41
1:B:644:LEU:HD12	1:B:645:CYS:N	2.35	0.41
1:B:873:ASP:HB3	1:B:876:GLU:OE1	2.21	0.41
1:B:792:LEU:N	1:B:792:LEU:HD22	2.33	0.41
1:B:845:VAL:HG11	1:B:901:LEU:HD12	2.03	0.41
1:A:565:ILE:O	1:A:566:VAL:HG23	2.20	0.41
1:A:628:TYR:CD1	1:A:642:ILE:CG2	3.03	0.41
1:A:680:HIS:ND1	1:A:753:TYR:HB2	2.36	0.41
1:A:694:ILE:HG12	1:A:709:ILE:HG22	2.03	0.41
1:A:717:LYS:O	1:A:718:LEU:C	2.63	0.41
1:B:631:THR:O	1:B:632:GLU:HG2	2.20	0.41
1:B:633:LYS:HG3	1:B:634:ASP:O	2.21	0.41
1:B:661:LEU:CB	1:B:662:GLY:HA3	2.50	0.41
1:A:870:VAL:CG1	1:A:874:TRP:HB3	2.50	0.41
1:A:954:GLU:O	1:A:955:ARG:CB	2.69	0.41
1:B:583:GLY:O	1:B:585:ILE:HD12	2.20	0.41
1:B:837:LYS:HE3	1:B:959:THR:HG22	2.03	0.41
1:B:904:MET:CG	1:B:933:PHE:CE2	3.04	0.41
1:A:661:LEU:HD23	1:A:662:GLY:H	1.85	0.40
1:A:769:SER:OG	1:A:772:TYR:HB2	2.21	0.40
1:B:825:HIS:HD1	1:B:825:HIS:C	2.27	0.40
1:A:817:PRO:HA	1:A:820:ARG:HD3	2.03	0.40
1:B:572:CYS:SG	1:B:574:LYS:HB3	2.61	0.40
1:B:734:THR:O	1:B:735:GLU:C	2.61	0.40
1:B:898:ARG:HG3	1:B:899:ASP:N	2.35	0.40
1:A:775:PHE:O	1:A:784:ASN:HB2	2.21	0.40
1:A:769:SER:O	1:A:770:GLU:HB2	2.21	0.40
1:A:830:PRO:HG3	1:A:945:TYR:CD2	2.57	0.40
1:B:650:GLN:HG3	1:B:654:GLU:OE1	2.22	0.40
1:B:808:LEU:HB2	1:B:829:HIS:CE1	2.56	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:B:864:ARG:HH12	2:A:1001:31J:O24[4_545]	1.43	0.17
1:B:864:ARG:NH1	2:A:1001:31J:O24[4_545]	2.05	0.15

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	382/435 (88%)	321 (84%)	54 (14%)	7 (2%)	6	25
1	B	377/435 (87%)	329 (87%)	44 (12%)	4 (1%)	11	36
All	All	759/870 (87%)	650 (86%)	98 (13%)	11 (1%)	9	30

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	581	ALA
1	A	822	SER
1	B	925	ILE
1	B	592	ASP
1	A	656	LYS
1	A	907	LYS
1	A	888	LYS
1	A	958	GLN
1	B	866	GLY
1	B	565	ILE
1	A	732	PRO

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/387 (87%)	285 (85%)	52 (15%)	2	9
1	B	335/387 (87%)	274 (82%)	61 (18%)	2	6
All	All	672/774 (87%)	559 (83%)	113 (17%)	2	7

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	560	GLU
1	A	561	THR
1	A	566	VAL
1	A	568	LYS
1	A	598	VAL
1	A	599	LYS
1	A	600	ARG
1	A	604	GLU
1	A	616	LEU
1	A	634	ASP
1	A	636	GLN
1	A	638	GLN
1	A	640	ILE
1	A	649	LEU
1	A	656	LYS
1	A	661	LEU
1	A	663	LEU
1	A	668	LEU
1	A	681	SER
1	A	705	ILE
1	A	709	ILE
1	A	710	SER
1	A	731	VAL
1	A	738	ILE
1	A	752	THR
1	A	763	VAL
1	A	767	VAL
1	A	786	LEU
1	A	792	LEU
1	A	793	ASP
1	A	807	GLU
1	A	815	MET
1	A	820	ARG
1	A	825	HIS

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Mol	Chain	Res	Type
1	A	837	LYS
1	A	846	SER
1	A	848	ARG
1	A	855	ASP
1	A	878	ILE
1	A	879	THR
1	A	880	VAL
1	A	887	ARG
1	A	897	VAL
1	A	901	LEU
1	A	908	LYS
1	A	912	ARG
1	A	913	GLU
1	A	914	LEU
1	A	922	LEU
1	A	931	ARG
1	A	956	LEU
1	A	962	TRP
1	B	566	VAL
1	B	568	LYS
1	B	582	GLU
1	B	594	ARG
1	B	598	VAL
1	B	600	ARG
1	B	602	LEU
1	B	620	ASP
1	B	627	ARG
1	B	630	CYS
1	B	634	ASP
1	B	636	GLN
1	B	638	GLN
1	B	640	ILE
1	B	642	ILE
1	B	649	LEU
1	B	650	GLN
1	B	661	LEU
1	B	663	LEU
1	B	668	LEU
1	B	676	LEU
1	B	684	ILE
1	B	690	LYS
1	B	698	MET

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Mol	Chain	Res	Type
1	B	705	ILE
1	B	709	ILE
1	B	714	LEU
1	B	752	THR
1	B	767	VAL
1	B	792	LEU
1	B	807	GLU
1	B	809	ILE
1	B	811	LYS
1	B	815	MET
1	B	819	GLN
1	B	820	ARG
1	B	824	LYS
1	B	825	HIS
1	B	835	LEU
1	B	845	VAL
1	B	854	LEU
1	B	855	ASP
1	B	858	ILE
1	B	864	ARG
1	B	869	VAL
1	B	878	ILE
1	B	879	THR
1	B	880	VAL
1	B	887	ARG
1	B	893	LYS
1	B	898	ARG
1	B	901	LEU
1	B	905	ARG
1	B	912	ARG
1	B	916	VAL
1	B	922	LEU
1	B	927	ASP
1	B	935	SER
1	B	936	ARG
1	B	953	HIS
1	B	956	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	624	ASN

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Mol	Chain	Res	Type
1	A	655	GLN
1	A	693	ASN
1	A	702	HIS
1	A	773	HIS
1	A	819	GLN
1	A	877	ASN
1	A	883	GLN
1	A	939	HIS
1	B	624	ASN
1	B	692	HIS
1	B	693	ASN
1	B	819	GLN
1	B	838	GLN
1	B	877	ASN
1	B	906	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	ADP	A	1002	4	28,29,29	1.56	5 (17%)	43,45,45	1.97	15 (34%)
2	31J	B	1001	1	24,24,24	1.66	4 (16%)	30,33,33	2.96	14 (46%)
3	ADP	B	1002	4	28,29,29	1.42	4 (14%)	43,45,45	1.90	11 (25%)
2	31J	A	1001	1	24,24,24	1.59	1 (4%)	30,33,33	2.71	13 (43%)

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
3	ADP	A	1002	4	-	5/16/32/32	0/3/3/3
2	31J	B	1001	1	-	1/9/9/9	0/2/2/2
3	ADP	B	1002	4	-	4/16/32/32	0/3/3/3
2	31J	A	1001	1	-	2/9/9/9	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	31J	C08-C09	6.94	1.47	1.35
2	B	1001	31J	C08-C09	6.41	1.46	1.35
3	B	1002	ADP	C5-C4	4.82	1.47	1.39
3	A	1002	ADP	C5-C4	4.14	1.46	1.39
3	A	1002	ADP	PA-O3A	3.71	1.63	1.59
3	A	1002	ADP	C5-N7	-2.87	1.33	1.39
3	B	1002	ADP	C8-N7	2.84	1.37	1.31
3	A	1002	ADP	C8-N7	2.62	1.36	1.31
3	B	1002	ADP	C5-C6	2.56	1.48	1.41
3	A	1002	ADP	C4-N9	-2.54	1.32	1.37
2	B	1001	31J	C13-C16	-2.32	1.37	1.40
2	B	1001	31J	C16-C18	-2.22	1.35	1.40
2	B	1001	31J	C19-C18	-2.12	1.47	1.51
3	B	1002	ADP	C5-N7	-2.06	1.35	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	31J	O14-C13-C16	7.20	122.06	114.53
2	B	1001	31J	C11-C21-C18	-6.15	118.86	123.27
2	A	1001	31J	C11-C21-C18	-6.09	118.90	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	31J	O14-C13-C16	6.05	120.86	114.53
3	B	1002	ADP	C5-C4-N3	-5.96	118.50	126.72
2	B	1001	31J	O22-C21-C18	5.38	121.37	114.89
2	B	1001	31J	C19-C18-C16	-5.22	111.81	120.52
3	A	1002	ADP	C5-C4-N3	-4.97	119.87	126.72
3	B	1002	ADP	N3-C4-N9	4.63	135.04	127.17
2	A	1001	31J	C07-C08-C09	-4.48	119.23	124.19
2	B	1001	31J	C12-C11-C09	-4.16	118.08	123.17
2	B	1001	31J	C19-C18-C21	4.15	127.72	121.24
2	B	1001	31J	C23-C08-C09	-4.12	117.48	120.35
3	B	1002	ADP	C2-N3-C4	4.04	121.69	111.83
3	A	1002	ADP	N3-C4-N9	3.99	133.95	127.17
2	A	1001	31J	C23-C08-C09	-3.98	117.58	120.35
3	B	1002	ADP	N3-C2-N1	-3.85	122.75	128.58
3	A	1002	ADP	O4'-C1'-N9	3.84	115.47	108.09
3	A	1002	ADP	N3-C2-N1	-3.63	123.08	128.58
2	A	1001	31J	O22-C21-C18	3.62	119.24	114.89
2	B	1001	31J	O24-C23-C08	-3.51	117.35	125.55
2	B	1001	31J	O22-C23-O24	3.51	120.84	116.22
2	A	1001	31J	C12-C11-C09	-3.44	118.96	123.17
3	A	1002	ADP	C2-N3-C4	3.43	120.21	111.83
2	A	1001	31J	O14-C13-C12	-3.40	118.22	124.08
2	B	1001	31J	C21-C11-C09	3.32	121.98	118.63
3	A	1002	ADP	O3B-PB-O3A	-3.25	93.73	104.64
2	B	1001	31J	O22-C23-C08	3.17	121.81	117.86
2	B	1001	31J	C10-C09-C11	3.13	122.06	118.49
2	B	1001	31J	O14-C13-C12	-3.13	118.69	124.08
2	A	1001	31J	C10-C09-C11	3.07	121.99	118.49
3	B	1002	ADP	C3'-C2'-C1'	3.05	107.23	101.46
3	B	1002	ADP	C4-C5-N7	-2.88	107.29	110.58
3	A	1002	ADP	O2A-PA-O3A	2.71	114.60	107.27
2	B	1001	31J	C16-C18-C21	2.67	120.46	116.86
3	A	1002	ADP	C4-N9-C8	2.67	108.54	105.74
2	A	1001	31J	C16-C18-C21	2.65	120.43	116.86
2	A	1001	31J	C07-C08-C23	2.63	123.18	117.15
3	A	1002	ADP	C2'-C1'-N9	-2.57	106.92	113.30
2	A	1001	31J	O24-C23-C08	-2.53	119.65	125.55
2	A	1001	31J	O22-C23-O24	2.52	119.54	116.22
3	A	1002	ADP	N9-C8-N7	-2.38	110.56	113.94
2	A	1001	31J	O22-C23-C08	2.37	120.81	117.86
3	B	1002	ADP	C4-N9-C8	2.30	108.16	105.74
3	B	1002	ADP	O3B-PB-O2B	2.26	116.27	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	ADP	O3B-PB-O2B	2.25	116.23	107.80
3	A	1002	ADP	O3A-PA-O1A	-2.23	104.00	110.70
3	A	1002	ADP	C4-C5-N7	-2.23	108.04	110.58
3	B	1002	ADP	C5-N7-C8	2.19	106.89	103.45
3	A	1002	ADP	N6-C6-N1	2.13	123.12	118.38
3	B	1002	ADP	C6-C5-N7	2.06	136.06	132.09
3	A	1002	ADP	C5-N7-C8	2.05	106.67	103.45
3	B	1002	ADP	O5'-C5'-C4'	2.01	115.84	108.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	ADP	C5'-O5'-PA-O2A
3	A	1002	ADP	C5'-O5'-PA-O3A
3	A	1002	ADP	O4'-C4'-C5'-O5'
3	B	1002	ADP	O4'-C4'-C5'-O5'
3	B	1002	ADP	C3'-C4'-C5'-O5'
3	A	1002	ADP	C3'-C4'-C5'-O5'
2	A	1001	31J	O02-C03-C04-O05
3	B	1002	ADP	PB-O3A-PA-O1A
2	B	1001	31J	C04-C03-O02-C01
3	A	1002	ADP	C5'-O5'-PA-O1A
3	B	1002	ADP	PB-O3A-PA-O2A
2	A	1001	31J	C04-C03-O02-C01

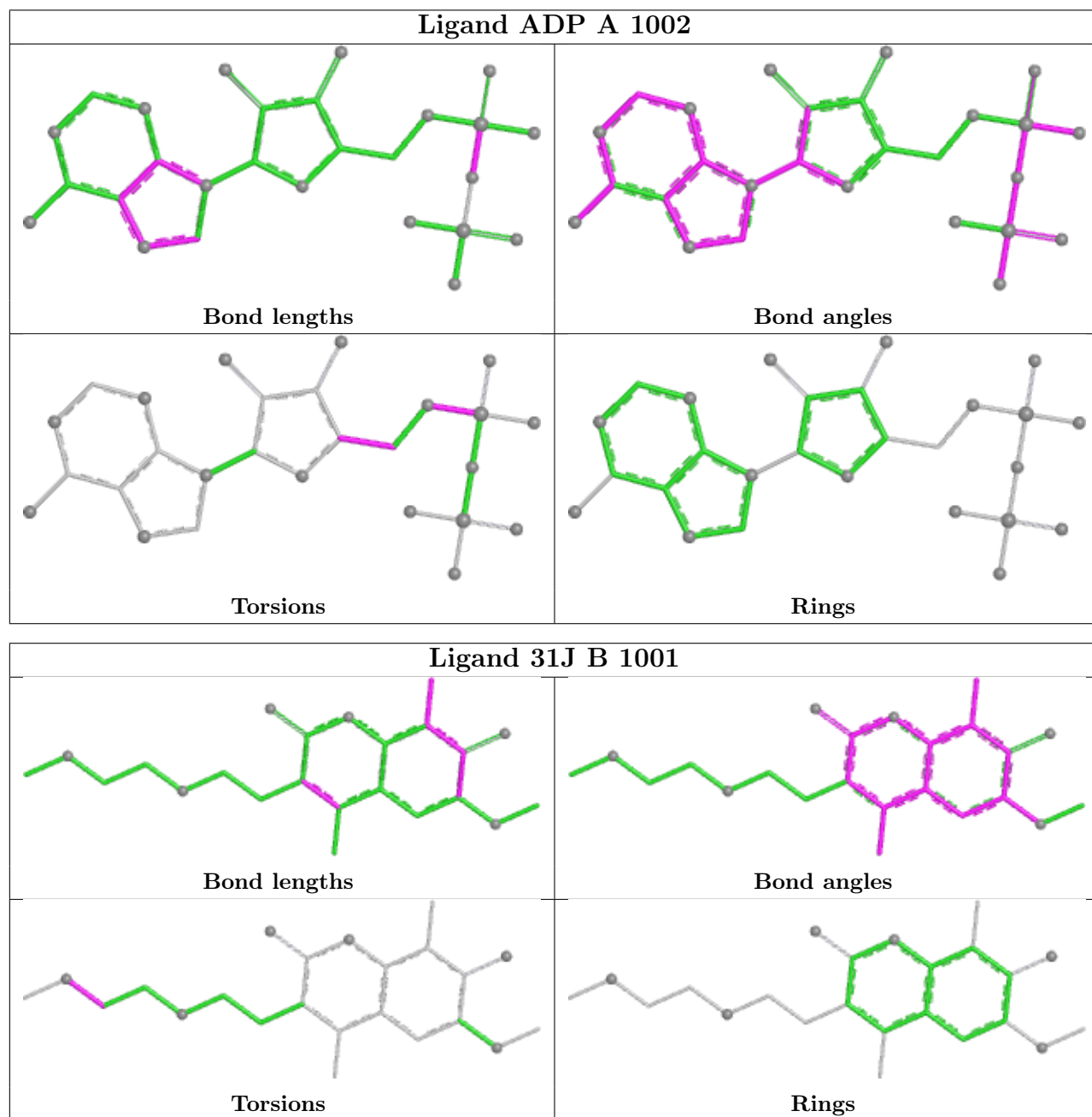
There are no ring outliers.

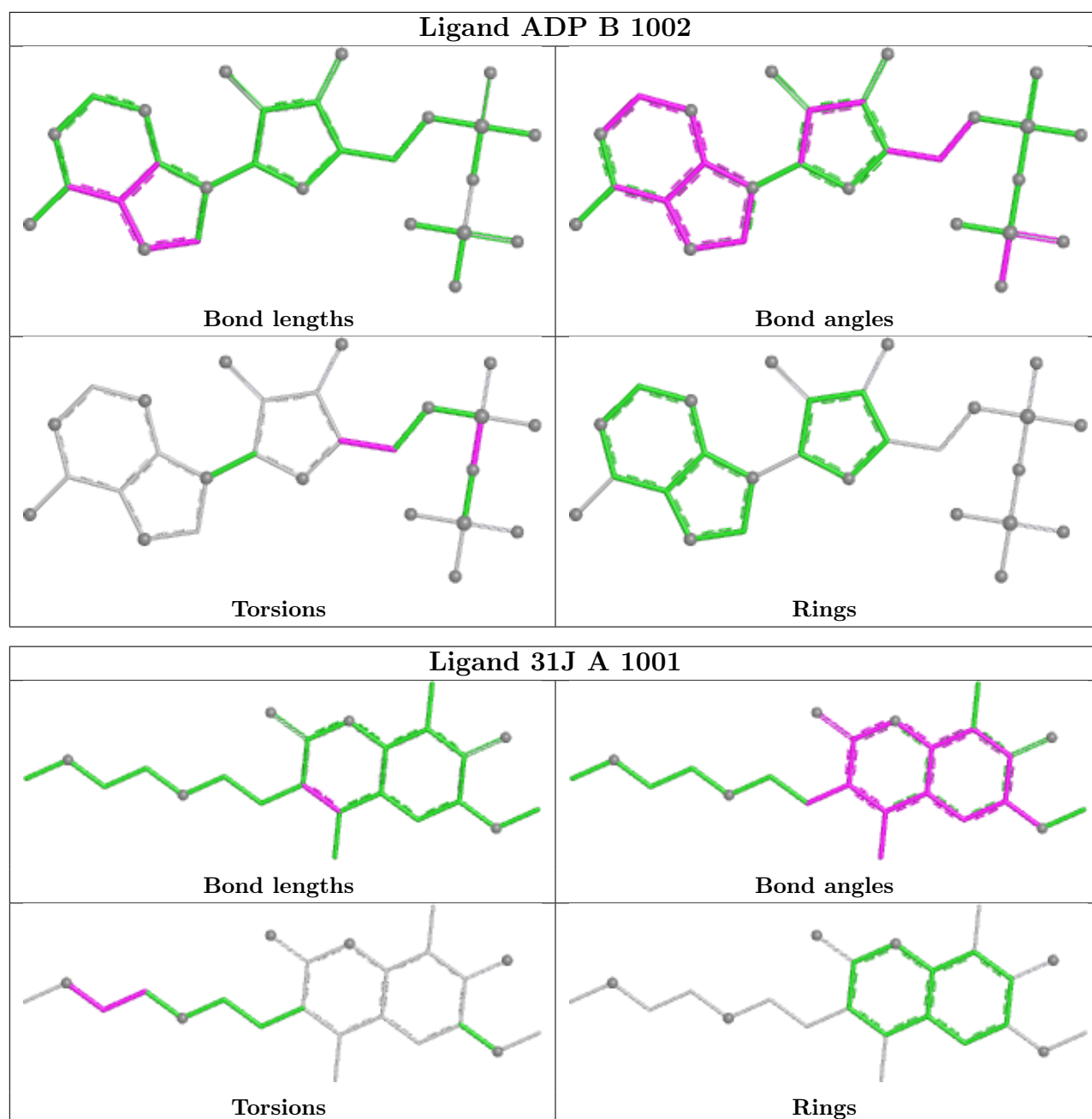
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	ADP	5	0
3	B	1002	ADP	2	0
2	A	1001	31J	6	2

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 ⓘ

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	388/435 (89%)	0.87	48 (12%)	8 7	17, 44, 90, 114	0
1	B	383/435 (88%)	0.86	49 (12%)	7 6	20, 46, 84, 122	0
All	All	771/870 (88%)	0.86	97 (12%)	8 6	17, 45, 88, 122	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	963	HIS	6.1
1	B	731	VAL	6.0
1	A	731	VAL	5.7
1	B	851	LYS	5.6
1	A	614	GLN	5.2
1	A	718	LEU	5.1
1	A	962	TRP	4.8
1	A	924	SER	4.6
1	B	701	ALA	4.6
1	B	562	ARG	4.5
1	A	732	PRO	4.5
1	B	962	TRP	4.5
1	A	964	GLU	4.3
1	A	855	ASP	4.1
1	B	862	LEU	3.8
1	A	963	HIS	3.7
1	A	610	ASP	3.7
1	B	953	HIS	3.7
1	A	891	THR	3.5
1	A	890	ARG	3.5
1	B	946	GLN	3.4
1	B	715	CYS	3.4
1	A	620	ASP	3.4
1	B	819	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	955	ARG	3.4
1	B	742	MET	3.3
1	A	953	HIS	3.2
1	A	854	LEU	3.2
1	A	628	TYR	3.2
1	B	614	GLN	3.1
1	B	657	ASP	3.1
1	A	849	ILE	3.0
1	A	608	PHE	3.0
1	B	732	PRO	2.9
1	B	955	ARG	2.9
1	A	562	ARG	2.9
1	A	702	HIS	2.9
1	A	923	GLY	2.8
1	A	612	GLU	2.8
1	B	753	TYR	2.8
1	B	860	ARG	2.8
1	B	567	GLY	2.8
1	A	961	TYR	2.8
1	B	581	ALA	2.8
1	B	662	GLY	2.7
1	B	744	SER	2.7
1	B	949	GLU	2.7
1	A	561	THR	2.7
1	A	743	LEU	2.7
1	A	715	CYS	2.7
1	A	657	ASP	2.7
1	A	701	ALA	2.6
1	B	751	PRO	2.6
1	A	733	GLY	2.6
1	A	595	ASP	2.6
1	A	751	PRO	2.6
1	A	593	ASN	2.6
1	B	856	GLY	2.6
1	B	867	ARG	2.5
1	B	822	SER	2.5
1	A	888	LYS	2.5
1	B	660	HIS	2.5
1	B	702	HIS	2.4
1	B	594	ARG	2.4
1	B	717	LYS	2.4
1	A	902	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	658	PHE	2.4
1	B	664	GLU	2.4
1	B	807	GLU	2.4
1	B	566	VAL	2.3
1	A	750	ASN	2.3
1	A	867	ARG	2.3
1	B	563	MET	2.3
1	A	717	LYS	2.3
1	B	687	ARG	2.2
1	B	855	ASP	2.2
1	B	872	MET	2.2
1	A	656	LYS	2.2
1	B	716	LYS	2.2
1	A	776	GLY	2.2
1	A	932	TYR	2.2
1	A	889	PHE	2.2
1	B	658	PHE	2.2
1	B	659	ALA	2.2
1	B	852	GLU	2.2
1	B	617	ARG	2.1
1	B	861	GLN	2.1
1	B	793	ASP	2.1
1	A	749	ASP	2.1
1	B	890	ARG	2.1
1	A	735	GLU	2.1
1	A	713	GLY	2.1
1	B	778	SER	2.1
1	A	950	LEU	2.1
1	B	754	THR	2.1
1	B	923	GLY	2.0
1	A	819	GLN	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 ⓘ

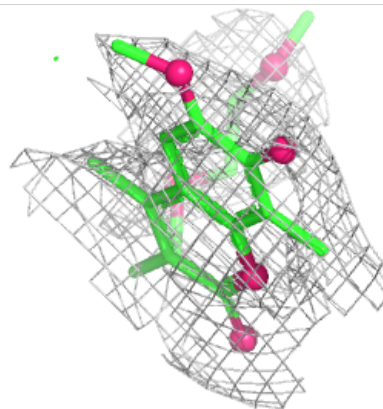
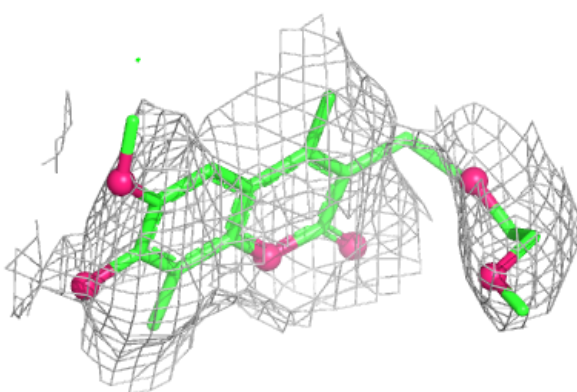
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	31J	A	1001	23/23	0.92	0.16	13,78,83,91	0
4	MG	A	1003	1/1	0.92	0.09	31,31,31,31	0
2	31J	B	1001	23/23	0.93	0.15	11,45,59,69	0
4	MG	B	1003	1/1	0.93	0.12	59,59,59,59	0
3	ADP	A	1002	27/27	0.95	0.09	20,20,24,24	0
3	ADP	B	1002	27/27	0.95	0.10	10,37,71,89	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.

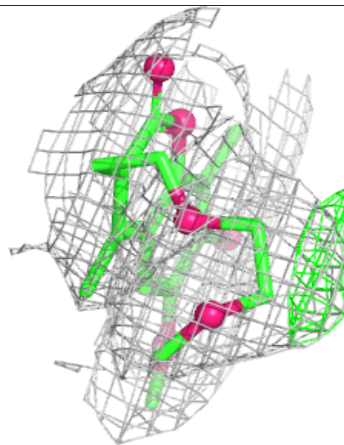
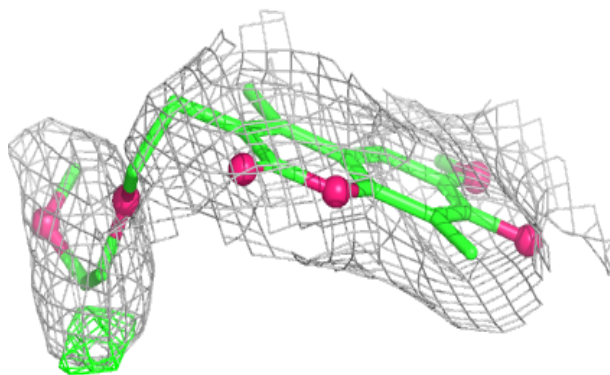
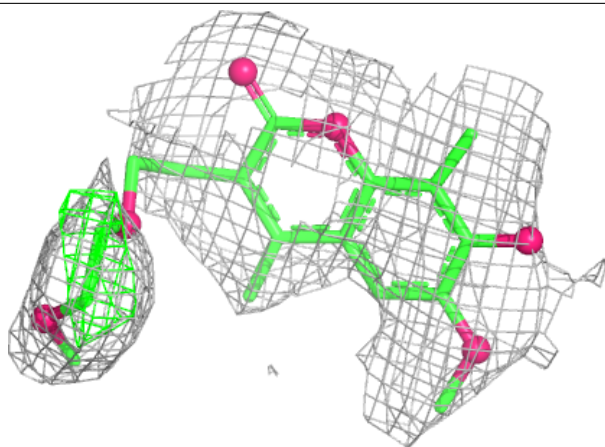
Electron density around 31J A 1001:

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



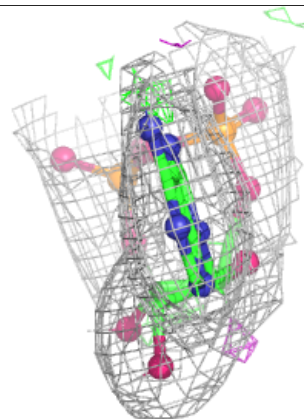
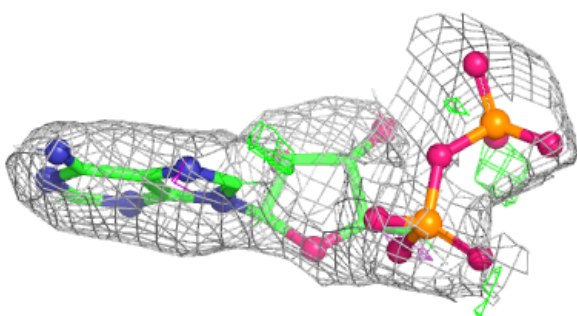
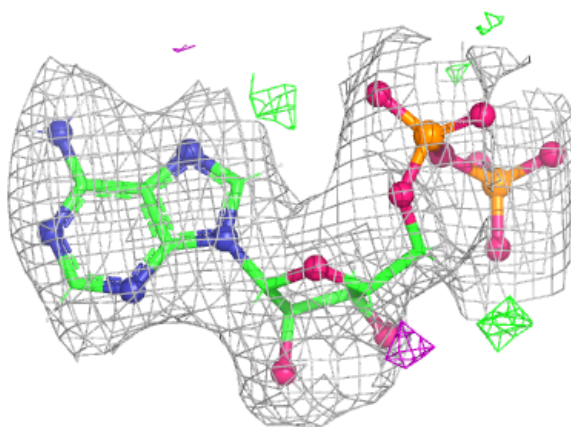
Electron density around 31J B 1001:

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

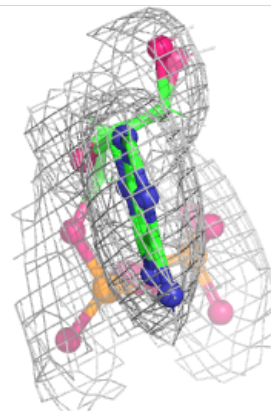
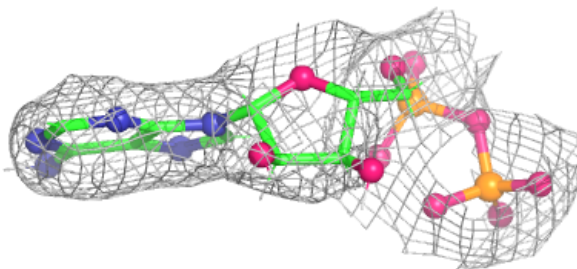
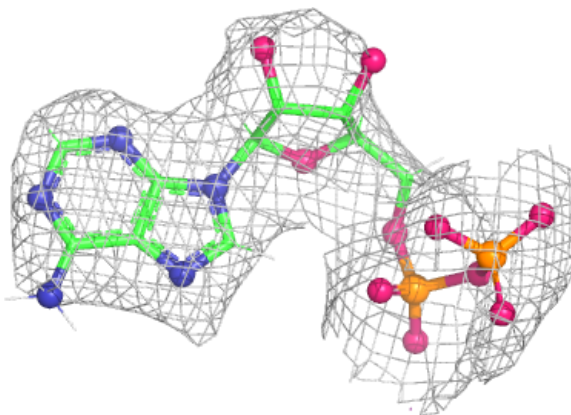


Electron density around ADP A 1002:

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

**Electron density around ADP B 1002:**

$2mF_o-DF_c$ (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.