



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 AM UTC

PDB ID : 4PL4 / pdb_00004pl4
Title : Crystal structure of murine IRE1 in complex with OICR464 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 : 3.00 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:

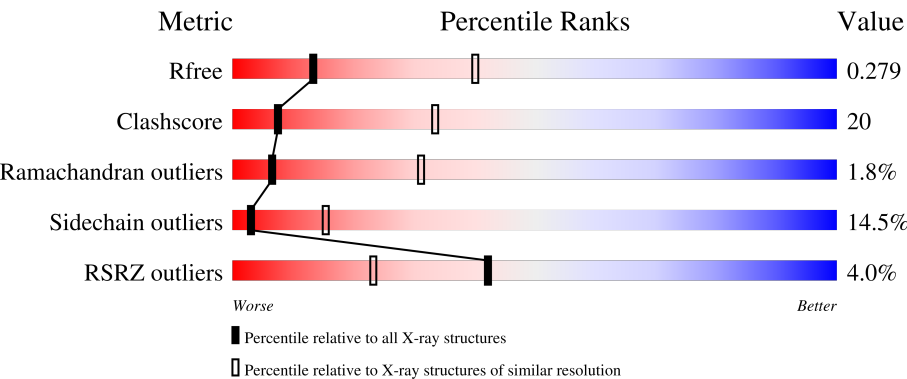
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	5% 47% 34% 7% 11%
1	B	435	2% 47% 33% 8% 12%
1	C	435	3% 53% 29% 6% 12%
1	D	435	5% 41% 36% 10% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12484 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3085	1976	537	553	19			
1	B	384	Total	C	N	O	S	0	0	0
			3104	1987	542	556	19			
1	C	384	Total	C	N	O	S	0	0	0
			3112	1992	547	554	19			
1	D	377	Total	C	N	O	S	0	0	0
			3031	1941	529	542	19			

There are 32 discrepancies between the modelled and reference sequences:

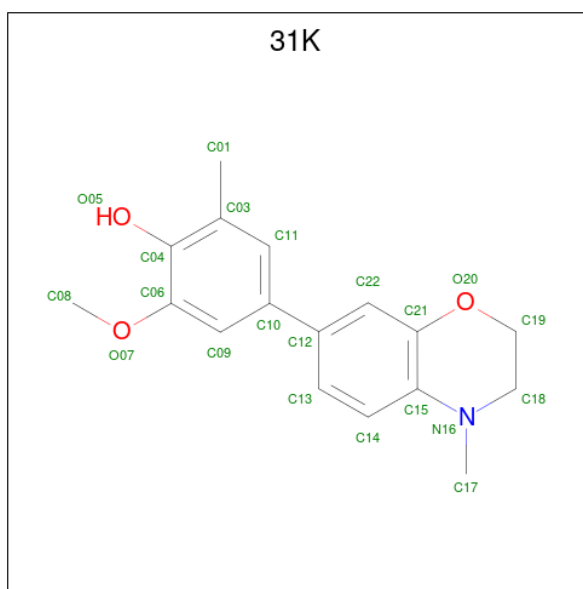
Chain	Residue	Modelled	Actual	Comment	Reference
A	543	GLY	-	expression tag	UNP Q9EQY0
A	544	ALA	-	expression tag	UNP Q9EQY0
A	545	MET	-	expression tag	UNP Q9EQY0
A	546	ASP	-	expression tag	UNP Q9EQY0
A	547	PRO	-	expression tag	UNP Q9EQY0
A	548	GLU	-	expression tag	UNP Q9EQY0
A	549	PHE	-	expression tag	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
C	543	GLY	-	expression tag	UNP Q9EQY0
C	544	ALA	-	expression tag	UNP Q9EQY0
C	545	MET	-	expression tag	UNP Q9EQY0
C	546	ASP	-	expression tag	UNP Q9EQY0
C	547	PRO	-	expression tag	UNP Q9EQY0

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

- Molecule 2 is 2-methoxy-6-methyl-4-(4-methyl-3,4-dihydro-2H-1,4-benzoxazin-7-yl)phenol (CCD ID: 31K) (formula: C₁₇H₁₉NO₃).



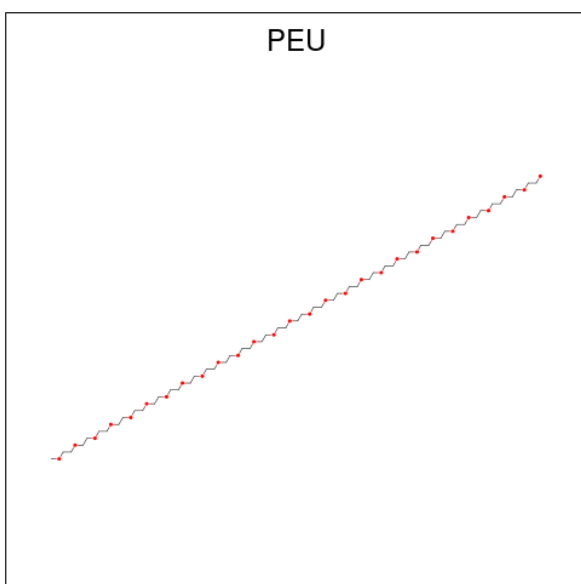
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	17	1	3		

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



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

- Molecule 4 is 2,5,8,11,14,17,20,23,26,29,32,35,38,41,44,47,50,53,56,59,62,65,68,71,74,77,80-H EPTACOSAODOCTACONTAN-82-OL (CCD ID: PEU) (formula: $C_{55}H_{112}O_{28}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

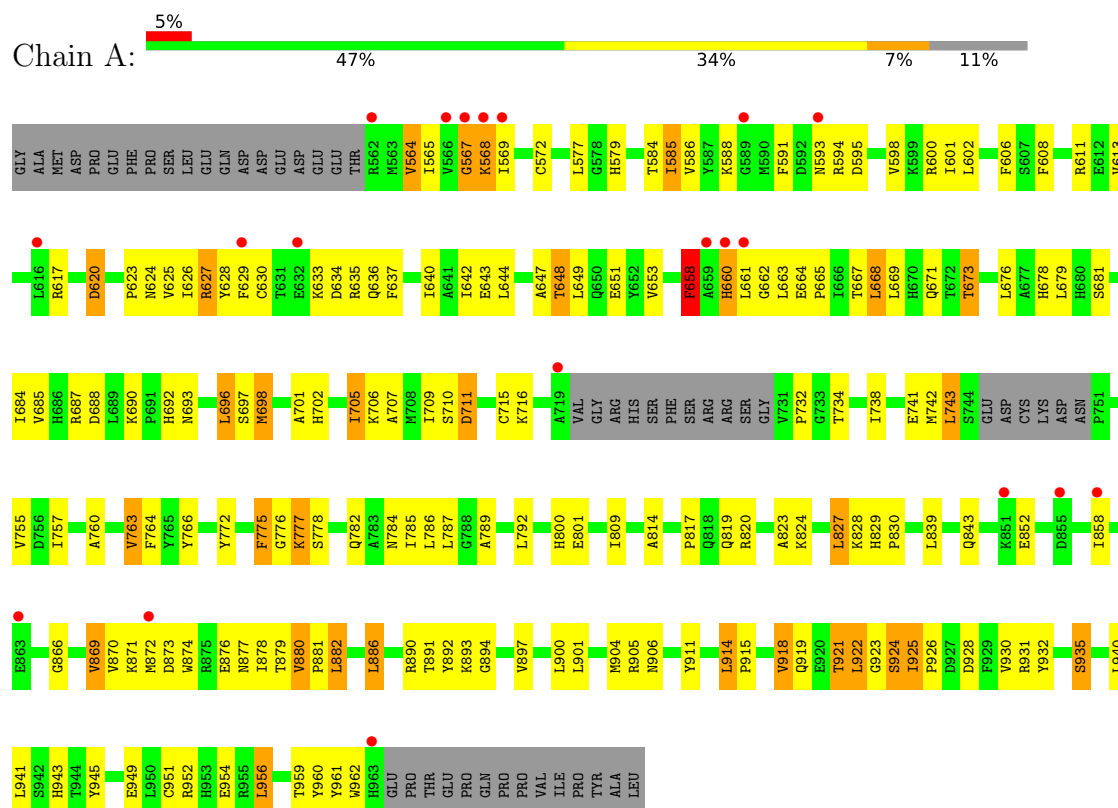
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

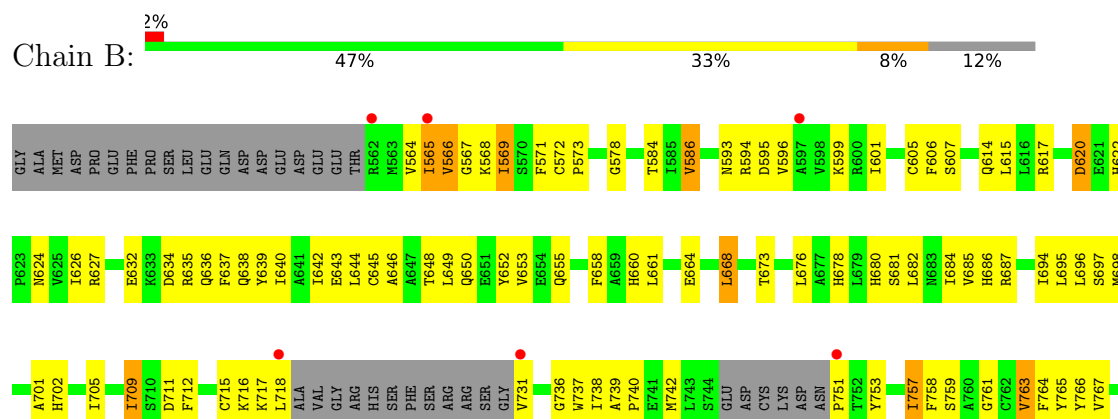
3 Residue-property plots

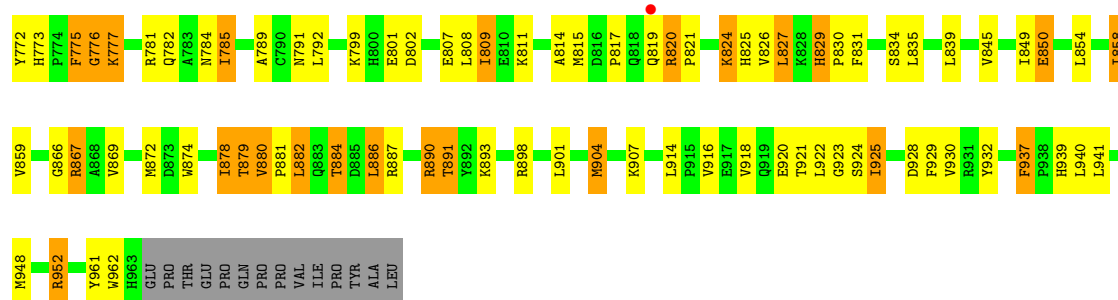
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

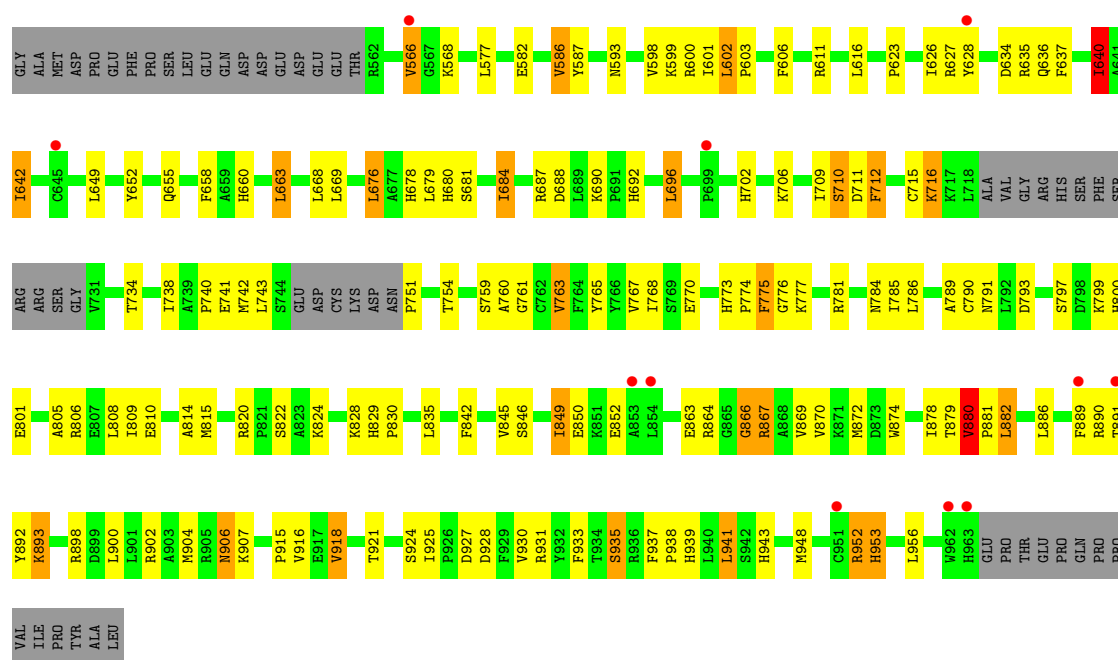


- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

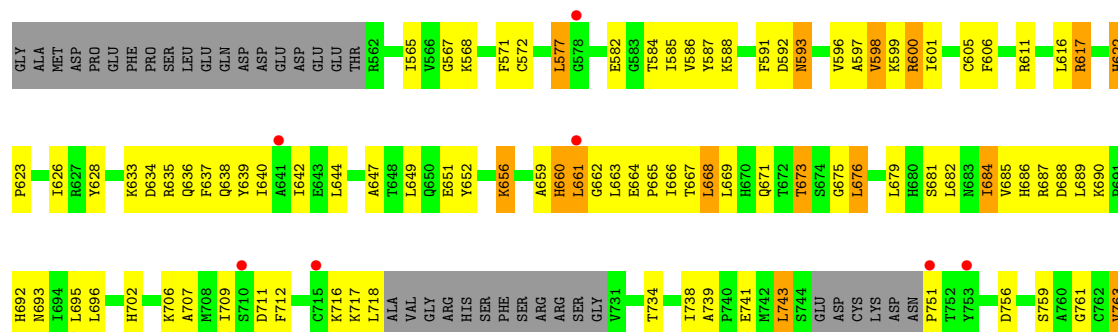


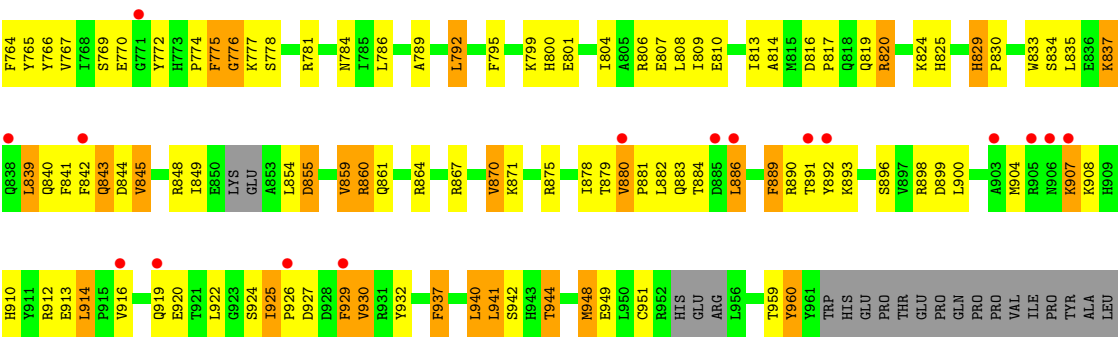


- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	319.11Å 62.31Å 141.33Å 90.00° 99.57° 90.00°	Depositor
Resolution (Å)	46.60 – 3.00 46.60 – 3.00	Depositor EDS
% Data completeness (in resolution range)	72.1 (46.60-3.00) 72.1 (46.60-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1175)	Depositor
R, R_{free}	0.210 , 0.276 0.214 , 0.279	Depositor DCC
R_{free} test set	2015 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.3	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	0.89	EDS
Total number of atoms	12484	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 31K, MG, PEU, 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	0.50	0/3162	0.95	9/4278 (0.2%)
1	B	0.49	1/3181 (0.0%)	0.95	11/4300 (0.3%)
1	C	0.47	1/3190 (0.0%)	0.93	6/4311 (0.1%)
1	D	0.48	0/3103	0.99	12/4191 (0.3%)
All	All	0.49	2/12636 (0.0%)	0.95	38/17080 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	880	VAL	CA-CB	6.98	1.58	1.54
1	B	880	VAL	CA-CB	6.54	1.57	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	775	PHE	N-CA-C	8.35	122.77	112.59
1	B	829	HIS	CA-C-N	7.99	129.83	119.84
1	B	829	HIS	C-N-CA	7.99	129.83	119.84
1	D	775	PHE	N-CA-C	7.98	124.00	113.30
1	A	658	PHE	N-CA-C	-7.97	102.62	113.30
1	D	572	CYS	CA-C-N	7.61	127.32	119.56
1	D	572	CYS	C-N-CA	7.61	127.32	119.56
1	B	775	PHE	N-CA-C	7.34	124.32	114.12
1	D	660	HIS	N-CA-C	6.89	118.58	111.14
1	D	647	ALA	N-CA-C	6.66	117.37	108.38
1	A	775	PHE	N-CA-C	6.48	123.43	113.19
1	D	622	HIS	CA-C-N	6.41	126.53	119.87
1	D	622	HIS	C-N-CA	6.41	126.53	119.87
1	A	567	GLY	N-CA-C	6.27	120.83	111.18
1	C	593	ASN	N-CA-C	-6.10	105.14	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	698	MET	CA-C-N	6.05	127.40	119.84
1	A	698	MET	C-N-CA	6.05	127.40	119.84
1	B	664	GLU	CA-C-N	5.97	125.45	119.24
1	B	664	GLU	C-N-CA	5.97	125.45	119.24
1	B	595	ASP	N-CA-C	-5.60	102.60	110.50
1	B	937	PHE	CA-C-N	5.58	125.25	119.05
1	B	937	PHE	C-N-CA	5.58	125.25	119.05
1	B	891	THR	N-CA-C	5.48	126.35	111.00
1	D	937	PHE	CA-C-N	5.38	124.72	118.85
1	D	937	PHE	C-N-CA	5.38	124.72	118.85
1	A	572	CYS	CA-C-N	5.32	124.99	119.56
1	A	572	CYS	C-N-CA	5.32	124.99	119.56
1	C	937	PHE	CA-C-N	5.29	125.35	119.32
1	C	937	PHE	C-N-CA	5.29	125.35	119.32
1	D	778	SER	N-CA-C	5.29	117.47	111.02
1	D	829	HIS	CA-C-N	5.24	124.96	119.82
1	D	829	HIS	C-N-CA	5.24	124.96	119.82
1	C	640	ILE	N-CA-C	5.22	115.63	108.12
1	A	660	HIS	N-CA-C	5.21	117.64	111.33
1	A	778	SER	N-CA-C	5.07	117.47	111.33
1	C	761	GLY	N-CA-C	-5.03	106.40	112.49
1	B	890	ARG	CA-C-N	5.00	130.70	121.70
1	B	890	ARG	C-N-CA	5.00	130.70	121.70

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	3085	0	3007	115	0
1	B	3104	0	3046	127	0
1	C	3112	0	3060	103	0
1	D	3031	0	2978	168	0
2	A	21	0	16	0	0
3	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
4	A	19	0	24	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	12484	0	12179	501	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 20.

All (501) 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:D:890:ARG:HB3	1:D:891:THR:HA	1.58	0.86
1:D:848:ARG:NH1	1:D:951:CYS:SG	2.50	0.85
1:C:867:ARG:NH1	1:D:810:GLU:OE2	2.10	0.84
1:B:652:TYR:HD2	1:B:696:LEU:HD11	1.43	0.83
1:A:623:PRO:O	1:A:706:LYS:NZ	2.12	0.81
1:A:911:TYR:HA	1:A:914:LEU:HD22	1.63	0.81
1:B:680:HIS:CE1	1:B:753:TYR:HB2	2.16	0.80
1:A:600:ARG:HE	1:A:637:PHE:HE2	1.26	0.80
1:A:568:LYS:HE3	1:A:591:PHE:HE1	1.47	0.79
1:B:614:GLN:HB2	1:B:617:ARG:HH21	1.48	0.79
1:A:620:ASP:OD1	1:A:620:ASP:N	2.11	0.78
1:D:817:PRO:HA	1:D:820:ARG:HG3	1.65	0.78
1:C:810:GLU:OE1	1:D:867:ARG:NH1	2.17	0.77
1:C:655:GLN:HB2	1:C:658:PHE:HB2	1.64	0.77
1:D:849:ILE:HG21	1:D:898:ARG:HE	1.50	0.77
1:A:900:LEU:HG	1:A:904:MET:HE2	1.68	0.76
1:A:627:ARG:HH11	1:A:643:GLU:HG2	1.47	0.76
1:D:814:ALA:O	1:D:820:ARG:NH1	2.18	0.76
1:D:693:ASN:HD21	1:D:711:ASP:HB2	1.51	0.74
1:B:655:GLN:HG3	1:B:658:PHE:HB2	1.70	0.74
1:D:854:LEU:HD12	1:D:859:VAL:HG21	1.68	0.74
1:B:620:ASP:OD1	1:B:620:ASP:N	2.18	0.73
1:A:701:ALA:HB1	1:B:565:ILE:HD11	1.70	0.72
1:D:855:ASP:OD1	1:D:855:ASP:N	2.22	0.71
1:C:791:ASN:ND2	1:C:793:ASP:OD2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:LYS:HD2	1:B:914:LEU:HD21	1.72	0.69
1:D:663:LEU:HD12	1:D:671:GLN:HE22	1.56	0.68
1:B:825:HIS:HD1	1:B:962:TRP:CD1	2.11	0.68
1:D:669:LEU:O	1:D:673:THR:HG23	1.94	0.68
1:A:627:ARG:NH1	1:A:643:GLU:HG2	2.09	0.67
1:B:615:LEU:HG	1:B:682:LEU:HD23	1.77	0.67
1:D:916:VAL:HG13	1:D:919:GLN:HG3	1.76	0.67
1:A:880:VAL:HG23	1:A:881:PRO:HD3	1.76	0.67
1:C:712:PHE:HD1	1:C:712:PHE:H	1.41	0.67
1:A:801:GLU:OE1	1:A:801:GLU:N	2.26	0.67
1:A:828:LYS:HD3	1:A:961:TYR:C	2.18	0.67
1:B:879:THR:OG1	1:B:932:TYR:OH	2.12	0.66
1:A:870:VAL:HG13	1:A:874:TRP:HB3	1.76	0.66
1:A:577:LEU:HB2	1:A:586:VAL:HG12	1.77	0.66
1:C:849:ILE:HD12	1:C:898:ARG:HG3	1.78	0.65
1:D:941:LEU:HD13	1:D:942:SER:N	2.10	0.65
1:A:565:ILE:HG22	1:A:567:GLY:H	1.60	0.65
1:D:834:SER:N	1:D:837:LYS:HZ1	1.94	0.65
1:B:622:HIS:HE1	1:B:624:ASN:HD22	1.43	0.65
1:D:922:LEU:HD23	1:D:929:PHE:HD2	1.62	0.64
1:D:835:LEU:HD12	1:D:835:LEU:H	1.62	0.64
1:D:914:LEU:HD11	1:D:919:GLN:CD	2.23	0.64
1:B:879:THR:HG1	1:B:932:TYR:HH	1.42	0.64
1:D:661:LEU:N	1:D:662:GLY:HA3	2.12	0.64
1:B:652:TYR:CD2	1:B:696:LEU:HD11	2.31	0.64
1:C:600:ARG:HB2	1:C:637:PHE:HD2	1.62	0.63
1:D:587:TYR:HB2	1:D:598:VAL:HG13	1.80	0.63
1:B:773:HIS:HD2	1:B:775:PHE:H	1.45	0.63
1:B:835:LEU:HD12	1:B:835:LEU:H	1.64	0.63
1:A:956:LEU:H	1:A:956:LEU:HD23	1.62	0.63
1:C:687:ARG:HD3	1:C:751:PRO:HG3	1.81	0.63
1:B:914:LEU:HD23	1:B:918:VAL:HG11	1.81	0.62
1:B:824:LYS:HA	1:B:827:LEU:HD12	1.81	0.62
1:B:901:LEU:HA	1:B:904:MET:HE3	1.81	0.62
1:C:906:ASN:OD1	1:C:907:LYS:NZ	2.30	0.62
1:D:634:ASP:OD1	1:D:635:ARG:N	2.33	0.61
1:D:636:GLN:HG2	1:D:637:PHE:HD1	1.64	0.61
1:B:565:ILE:HG23	1:B:566:VAL:H	1.65	0.61
1:C:586:VAL:HG13	1:C:599:LYS:HB3	1.83	0.61
1:A:923:GLY:HA2	1:A:924:SER:O	2.01	0.61
1:A:643:GLU:OE1	1:A:643:GLU:N	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:715:CYS:SG	1:C:716:LYS:N	2.74	0.61
1:A:901:LEU:HA	1:A:904:MET:HE3	1.82	0.61
1:C:690:LYS:NZ	1:C:734:THR:HG21	2.16	0.60
1:A:685:VAL:HG12	1:A:687:ARG:HG3	1.82	0.60
1:A:775:PHE:H	1:A:776:GLY:HA2	1.66	0.60
1:D:693:ASN:ND2	1:D:711:ASP:HB2	2.15	0.60
1:A:663:LEU:HD22	1:A:705:ILE:HG22	1.82	0.60
1:B:801:GLU:CD	1:B:801:GLU:H	2.09	0.60
1:C:866:GLY:O	1:C:869:VAL:HG12	2.02	0.60
1:D:622:HIS:CD2	1:D:623:PRO:HD2	2.36	0.60
1:A:648:THR:N	1:A:651:GLU:OE2	2.31	0.60
1:B:627:ARG:HH21	1:B:643:GLU:HG2	1.66	0.60
1:B:782:GLN:HA	1:B:785:ILE:HG23	1.83	0.60
1:A:715:CYS:SG	1:A:716:LYS:N	2.75	0.60
1:C:850:GLU:OE2	1:C:902:ARG:NH2	2.35	0.60
1:D:636:GLN:HG2	1:D:637:PHE:CD1	2.36	0.60
1:D:886:LEU:HB3	1:D:890:ARG:NH1	2.17	0.60
1:D:910:HIS:HA	1:D:912:ARG:HH12	1.67	0.60
1:A:661:LEU:N	1:A:662:GLY:HA3	2.17	0.59
1:D:690:LYS:HG2	1:D:693:ASN:HB2	1.84	0.59
1:D:926:PRO:O	1:D:930:VAL:HG22	2.02	0.59
1:B:758:PHE:HZ	1:B:775:PHE:HE2	1.50	0.59
1:D:844:ASP:OD2	1:D:960:TYR:OH	2.14	0.59
1:A:660:HIS:N	1:A:661:LEU:HA	2.17	0.59
1:C:741:GLU:OE2	1:C:820:ARG:NH2	2.36	0.59
1:D:839:LEU:HD23	1:D:930:VAL:HG13	1.84	0.59
1:A:904:MET:HE1	1:A:940:LEU:HD21	1.85	0.59
1:B:584:THR:HG21	1:B:599:LYS:HE3	1.85	0.59
1:B:775:PHE:CD2	1:B:785:ILE:HB	2.38	0.59
1:B:799:LYS:NZ	1:B:802:ASP:OD1	2.30	0.59
1:C:600:ARG:HB2	1:C:637:PHE:CD2	2.38	0.59
1:D:830:PRO:HA	1:D:833:TRP:CE2	2.38	0.59
1:D:634:ASP:HB2	1:D:639:TYR:HE1	1.67	0.58
1:D:666:ILE:H	1:D:666:ILE:HD12	1.68	0.58
1:D:599:LYS:HB3	1:D:640:ILE:HG23	1.85	0.58
1:C:623:PRO:O	1:C:706:LYS:NZ	2.29	0.58
1:C:784:ASN:HB3	1:C:789:ALA:HB3	1.84	0.58
1:A:873:ASP:HA	1:A:894:GLY:O	2.04	0.58
1:C:577:LEU:N	1:C:586:VAL:O	2.34	0.58
1:D:924:SER:O	1:D:925:ILE:HB	2.04	0.58
1:C:869:VAL:HG23	1:C:939:HIS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:ASN:HB3	1:A:789:ALA:HB3	1.86	0.57
1:D:834:SER:H	1:D:837:LYS:HZ1	1.50	0.57
1:A:601:ILE:HD12	1:A:606:PHE:HB2	1.85	0.57
1:C:678:HIS:O	1:C:681:SER:OG	2.17	0.57
1:B:569:ILE:HD13	1:B:569:ILE:H	1.69	0.57
1:D:880:VAL:HG23	1:D:881:PRO:HD3	1.87	0.57
1:B:678:HIS:O	1:B:681:SER:OG	2.14	0.56
1:B:758:PHE:CZ	1:B:785:ILE:HD13	2.41	0.56
1:A:928:ASP:HA	1:A:931:ARG:HG2	1.85	0.56
1:C:628:TYR:HD1	1:C:642:ILE:HG22	1.69	0.56
1:D:886:LEU:HD12	1:D:889:PHE:HD2	1.70	0.56
1:C:893:LYS:HD2	1:C:893:LYS:N	2.19	0.56
1:A:600:ARG:NE	1:A:637:PHE:HE2	2.01	0.56
1:B:605:CYS:O	1:B:717:LYS:HG2	2.06	0.56
1:D:800:HIS:CD2	1:D:941:LEU:HD12	2.41	0.56
1:B:808:LEU:HD11	1:B:826:VAL:HG13	1.87	0.56
1:D:616:LEU:HD23	1:D:682:LEU:HD22	1.88	0.55
1:D:886:LEU:HD11	1:D:907:LYS:HG2	1.88	0.55
1:C:634:ASP:OD1	1:C:635:ARG:N	2.39	0.55
1:C:892:TYR:HE1	1:C:902:ARG:HD2	1.70	0.55
1:D:835:LEU:HB3	1:D:930:VAL:HG21	1.88	0.55
1:A:960:TYR:C	1:A:961:TYR:HD1	2.14	0.55
1:D:808:LEU:HD13	1:D:829:HIS:CD2	2.42	0.55
1:D:833:TRP:HB3	1:D:837:LYS:HZ1	1.72	0.55
1:B:879:THR:HB	1:B:881:PRO:HD2	1.87	0.55
1:B:904:MET:HE1	1:B:940:LEU:HD21	1.88	0.55
1:A:710:SER:OG	1:A:711:ASP:OD1	2.20	0.55
1:B:878:ILE:HD12	1:B:882:LEU:HD12	1.88	0.55
1:A:690:LYS:HG3	1:A:692:HIS:H	1.72	0.54
1:A:890:ARG:HA	1:A:892:TYR:N	2.22	0.54
1:C:808:LEU:HD13	1:C:829:HIS:CD2	2.42	0.54
1:A:839:LEU:HD23	1:A:926:PRO:HB3	1.89	0.54
1:C:601:ILE:HD12	1:C:606:PHE:HB2	1.89	0.54
1:D:922:LEU:HD23	1:D:929:PHE:CD2	2.42	0.54
1:B:872:MET:HA	1:B:872:MET:HE2	1.89	0.54
1:B:775:PHE:CE2	1:B:785:ILE:HB	2.43	0.54
1:C:890:ARG:HG3	1:C:891:THR:H	1.71	0.54
1:D:830:PRO:HA	1:D:833:TRP:CD2	2.42	0.54
1:A:949:GLU:HA	1:A:961:TYR:CE2	2.42	0.54
1:B:685:VAL:HG12	1:B:687:ARG:HG3	1.89	0.54
1:D:687:ARG:NH2	1:D:751:PRO:HG2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:765:TYR:O	1:D:769:SER:OG	2.22	0.54
1:B:784:ASN:HB3	1:B:789:ALA:HB3	1.90	0.54
1:D:626:ILE:HD12	1:D:695:LEU:HD12	1.90	0.54
1:D:571:PHE:HB3	1:D:598:VAL:HG11	1.90	0.54
1:D:601:ILE:HD12	1:D:606:PHE:HB2	1.90	0.54
1:D:854:LEU:HA	1:D:859:VAL:HG11	1.90	0.54
1:D:900:LEU:HG	1:D:904:MET:HE2	1.89	0.54
1:D:676:LEU:HD11	1:D:756:ASP:HB3	1.89	0.53
1:C:669:LEU:HD11	1:C:767:VAL:HG21	1.88	0.53
1:C:688:ASP:OD1	1:C:734:THR:HG23	2.08	0.53
1:C:924:SER:N	1:C:928:ASP:HB2	2.23	0.53
1:C:805:ALA:O	1:C:809:ILE:HG12	2.08	0.53
1:B:578:GLY:O	1:B:586:VAL:HG23	2.09	0.53
1:B:839:LEU:HB2	1:B:930:VAL:HB	1.91	0.53
1:D:929:PHE:HA	1:D:932:TYR:HB3	1.90	0.53
1:C:867:ARG:HH12	1:D:810:GLU:CD	2.10	0.53
1:D:886:LEU:HB3	1:D:890:ARG:HH12	1.73	0.53
1:B:634:ASP:OD1	1:B:635:ARG:N	2.42	0.53
1:D:910:HIS:HA	1:D:912:ARG:NH1	2.23	0.53
1:A:690:LYS:HD2	1:A:692:HIS:HB2	1.91	0.53
1:B:765:TYR:CE1	1:B:792:LEU:HA	2.44	0.53
1:A:952:ARG:NH2	1:A:962:TRP:O	2.36	0.53
1:B:839:LEU:HD13	1:B:930:VAL:HB	1.92	0.52
1:C:867:ARG:HH11	1:C:872:MET:HB3	1.74	0.52
1:C:886:LEU:HD13	1:C:889:PHE:HE2	1.75	0.52
1:A:775:PHE:N	1:A:776:GLY:HA2	2.23	0.52
1:B:694:ILE:HG12	1:B:709:ILE:HG22	1.92	0.52
1:C:867:ARG:HE	1:C:872:MET:HA	1.74	0.52
1:C:775:PHE:N	1:C:776:GLY:HA2	2.25	0.52
1:D:835:LEU:HD22	1:D:927:ASP:HA	1.91	0.52
1:A:760:ALA:HA	1:A:763:VAL:HG13	1.90	0.52
1:B:924:SER:H	1:B:928:ASP:HB2	1.74	0.52
1:C:879:THR:HG22	1:C:882:LEU:HB2	1.92	0.52
1:B:791:ASN:H	1:B:792:LEU:HD22	1.75	0.52
1:B:884:THR:HA	1:B:887:ARG:NH1	2.25	0.52
1:D:896:SER:HB3	1:D:899:ASP:HB2	1.92	0.52
1:D:577:LEU:HD21	1:D:644:LEU:HD11	1.91	0.51
1:D:690:LYS:HD2	1:D:692:HIS:HB2	1.92	0.51
1:A:678:HIS:O	1:A:681:SER:OG	2.16	0.51
1:A:925:ILE:HG13	1:A:926:PRO:HA	1.93	0.51
1:D:834:SER:O	1:D:837:LYS:NZ	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:940:LEU:O	1:D:944:THR:OG1	2.26	0.51
1:A:711:ASP:OD1	1:A:711:ASP:N	2.43	0.51
1:A:743:LEU:HD23	1:A:786:LEU:HD11	1.91	0.51
1:D:660:HIS:N	1:D:661:LEU:HA	2.24	0.51
1:A:915:PRO:O	1:A:919:GLN:HG3	2.10	0.51
1:B:614:GLN:HB2	1:B:617:ARG:NH2	2.22	0.51
1:B:849:ILE:HD11	1:B:948:MET:SD	2.50	0.51
1:A:594:ARG:HH12	1:B:593:ASN:H	1.58	0.51
1:B:858:ILE:HG23	1:B:859:VAL:H	1.74	0.51
1:C:880:VAL:HG13	1:C:881:PRO:HD3	1.92	0.50
1:B:773:HIS:CE1	1:B:781:ARG:HD3	2.46	0.50
1:B:814:ALA:O	1:B:820:ARG:NH1	2.45	0.50
1:D:834:SER:H	1:D:837:LYS:NZ	2.09	0.50
1:D:908:LYS:HE3	1:D:929:PHE:CZ	2.46	0.50
1:A:882:LEU:HD12	1:A:932:TYR:OH	2.12	0.50
1:A:931:ARG:O	1:A:935:SER:HB3	2.11	0.50
1:B:766:TYR:HA	1:B:772:TYR:O	2.10	0.50
1:B:764:PHE:HB3	1:B:809:ILE:HD13	1.93	0.50
1:C:676:LEU:HD22	1:C:680:HIS:CE1	2.47	0.50
1:D:565:ILE:HG22	1:D:567:GLY:H	1.77	0.50
1:A:800:HIS:HB3	1:A:801:GLU:OE1	2.11	0.50
1:D:833:TRP:HB3	1:D:837:LYS:NZ	2.27	0.50
1:B:601:ILE:HG13	1:B:638:GLN:HB3	1.93	0.50
1:B:849:ILE:HG22	1:B:898:ARG:HE	1.76	0.50
1:C:886:LEU:HD13	1:C:889:PHE:CE2	2.47	0.50
1:D:649:LEU:HD21	1:D:668:LEU:HD11	1.94	0.49
1:D:890:ARG:HA	1:D:892:TYR:H	1.76	0.49
1:D:840:GLN:HA	1:D:843:GLN:OE1	2.12	0.49
1:D:842:PHE:O	1:D:845:VAL:HG13	2.13	0.49
1:A:697:SER:OG	1:A:706:LYS:HG2	2.12	0.49
1:A:817:PRO:HA	1:A:820:ARG:HG3	1.94	0.49
1:D:741:GLU:OE2	1:D:820:ARG:NH2	2.46	0.49
1:D:849:ILE:CG2	1:D:898:ARG:HE	2.22	0.49
1:D:937:PHE:HB2	1:D:940:LEU:HD12	1.92	0.49
1:B:686:HIS:CD2	1:B:712:PHE:HB3	2.48	0.49
1:B:850:GLU:HA	1:B:898:ARG:NH2	2.27	0.49
1:A:634:ASP:OD1	1:A:635:ARG:N	2.46	0.49
1:C:800:HIS:HB2	1:C:938:PRO:HA	1.94	0.49
1:D:605:CYS:HB2	1:D:606:PHE:CD2	2.47	0.49
1:D:861:GLN:O	1:D:864:ARG:HB2	2.12	0.49
1:A:643:GLU:H	1:A:643:GLU:CD	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:CYS:HB3	1:B:696:LEU:O	2.13	0.49
1:C:814:ALA:O	1:C:820:ARG:NH1	2.45	0.49
1:D:795:PHE:HB3	1:D:806:ARG:HG3	1.95	0.49
1:D:808:LEU:HB2	1:D:829:HIS:CE1	2.47	0.49
1:A:568:LYS:HE2	1:A:569:ILE:HG13	1.95	0.49
1:A:649:LEU:O	1:A:653:VAL:HG23	2.13	0.49
1:B:599:LYS:HB3	1:B:640:ILE:HG23	1.95	0.48
1:D:882:LEU:HG	1:D:886:LEU:HD22	1.95	0.48
1:A:588:LYS:NZ	1:A:595:ASP:OD1	2.44	0.48
1:A:829:HIS:CG	1:A:830:PRO:HD2	2.48	0.48
1:A:871:LYS:HE3	1:A:877:ASN:OD1	2.13	0.48
1:B:773:HIS:CD2	1:B:775:PHE:H	2.29	0.48
1:D:568:LYS:HZ2	1:D:591:PHE:HZ	1.61	0.48
1:B:606:PHE:CE1	1:B:716:LYS:HG3	2.48	0.48
1:D:867:ARG:HA	1:D:870:VAL:HG23	1.95	0.48
1:A:951:CYS:HB3	1:A:954:GLU:CD	2.39	0.48
1:C:710:SER:OG	1:C:711:ASP:N	2.46	0.48
1:D:588:LYS:HG3	1:D:644:LEU:HD21	1.95	0.48
1:D:656:LYS:HD3	1:D:656:LYS:H	1.78	0.48
1:A:741:GLU:OE2	1:A:820:ARG:NH2	2.46	0.48
1:C:598:VAL:HA	1:C:640:ILE:O	2.12	0.48
1:A:949:GLU:HA	1:A:961:TYR:HE2	1.78	0.48
1:D:784:ASN:HB3	1:D:789:ALA:HB3	1.95	0.48
1:C:915:PRO:O	1:C:918:VAL:HG13	2.14	0.48
1:D:912:ARG:NH2	1:D:913:GLU:OE1	2.46	0.48
1:B:824:LYS:HB2	1:B:962:TRP:CH2	2.49	0.48
1:A:693:ASN:OD1	1:A:711:ASP:OD2	2.32	0.48
1:C:774:PRO:HB2	1:C:775:PHE:CD1	2.49	0.48
1:D:765:TYR:CE2	1:D:792:LEU:HA	2.49	0.48
1:D:860:ARG:O	1:D:864:ARG:HG3	2.14	0.48
1:D:937:PHE:O	1:D:940:LEU:HB2	2.14	0.48
1:A:569:ILE:HG21	1:A:598:VAL:HG11	1.96	0.47
1:C:924:SER:H	1:C:928:ASP:HB2	1.77	0.47
1:A:565:ILE:HD12	1:B:701:ALA:HB1	1.96	0.47
1:B:564:VAL:HG12	1:B:565:ILE:H	1.79	0.47
1:C:586:VAL:HG21	3:C:1001:ADP:O4'	2.14	0.47
1:B:649:LEU:HD11	1:B:767:VAL:HG22	1.96	0.47
1:B:777:LYS:C	1:B:781:ARG:HG3	2.39	0.47
1:D:687:ARG:CZ	1:D:751:PRO:HG2	2.44	0.47
1:D:824:LYS:HB2	1:D:824:LYS:HE3	1.56	0.47
1:A:594:ARG:HB3	1:B:594:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:LEU:HD13	1:A:764:PHE:CG	2.49	0.47
1:B:709:ILE:HD13	1:B:709:ILE:H	1.79	0.47
1:C:628:TYR:CD1	1:C:642:ILE:HG22	2.50	0.47
1:C:864:ARG:HE	1:D:864:ARG:HG2	1.80	0.47
1:C:867:ARG:HE	1:C:872:MET:CA	2.27	0.47
1:C:904:MET:HG2	1:C:933:PHE:CZ	2.50	0.47
1:C:952:ARG:HA	1:C:953:HIS:HA	1.70	0.47
1:D:626:ILE:HG22	1:D:712:PHE:HE1	1.79	0.47
1:D:775:PHE:CE1	1:D:813:ILE:HD12	2.50	0.47
1:B:773:HIS:ND1	1:B:781:ARG:HD3	2.29	0.47
1:C:801:GLU:CD	1:C:801:GLU:H	2.23	0.47
1:D:634:ASP:HB3	1:D:637:PHE:HB2	1.96	0.47
1:B:924:SER:O	1:B:925:ILE:HB	2.15	0.47
1:D:649:LEU:O	1:D:652:TYR:HB3	2.14	0.47
1:D:777:LYS:O	1:D:781:ARG:HG3	2.14	0.47
1:B:845:VAL:O	1:B:849:ILE:HG12	2.15	0.47
1:C:882:LEU:O	1:C:886:LEU:HD23	2.15	0.47
1:D:764:PHE:HB3	1:D:809:ILE:HD13	1.97	0.47
1:D:833:TRP:CH2	1:D:841:PHE:HD2	2.33	0.47
1:B:776:GLY:O	1:B:781:ARG:NH1	2.48	0.46
1:A:568:LYS:HE2	1:A:569:ILE:N	2.30	0.46
1:D:761:GLY:O	1:D:764:PHE:HB2	2.15	0.46
1:B:907:LYS:HA	1:B:907:LYS:HD3	1.52	0.46
1:D:804:ILE:HD11	1:D:941:LEU:HD11	1.97	0.46
1:D:652:TYR:HD2	1:D:696:LEU:HD11	1.79	0.46
1:D:799:LYS:HD2	1:D:799:LYS:HA	1.71	0.46
1:D:597:ALA:HB3	1:D:642:ILE:HG13	1.96	0.46
1:D:661:LEU:H	1:D:662:GLY:HA3	1.77	0.46
1:A:766:TYR:HA	1:A:772:TYR:O	2.15	0.46
1:A:873:ASP:HB3	1:A:876:GLU:HG2	1.98	0.46
1:B:652:TYR:CE2	1:B:668:LEU:HD12	2.50	0.46
1:B:808:LEU:HB2	1:B:829:HIS:NE2	2.31	0.46
1:D:679:LEU:HD22	1:D:709:ILE:HD12	1.98	0.46
1:A:564:VAL:O	1:A:565:ILE:HD13	2.16	0.46
1:D:880:VAL:O	1:D:884:THR:HG23	2.15	0.46
1:A:830:PRO:HG3	1:A:945:TYR:CE2	2.51	0.46
1:B:867:ARG:HB3	1:B:872:MET:CE	2.45	0.46
1:C:602:LEU:HA	1:C:603:PRO:HD3	1.82	0.46
1:D:706:LYS:HG2	1:D:707:ALA:H	1.79	0.46
1:B:634:ASP:HB3	1:B:637:PHE:HB2	1.98	0.46
1:C:759:SER:O	1:C:763:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:591:PHE:HB2	1:D:596:VAL:HG21	1.98	0.46
1:C:845:VAL:HG13	1:C:948:MET:HE2	1.97	0.46
1:D:882:LEU:O	1:D:886:LEU:HB2	2.16	0.46
1:A:611:ARG:HA	1:A:611:ARG:HD3	1.71	0.45
1:C:797:SER:HB3	1:D:871:LYS:HD3	1.98	0.45
1:D:584:THR:O	1:D:585:ILE:HD13	2.16	0.45
1:A:617:ARG:NH1	1:A:628:TYR:O	2.50	0.45
1:D:686:HIS:CE1	1:D:712:PHE:HB3	2.50	0.45
1:D:882:LEU:HD11	1:D:907:LYS:HG3	1.97	0.45
1:A:579:HIS:CE1	1:A:585:ILE:HD12	2.51	0.45
1:A:918:VAL:O	1:A:921:THR:HG22	2.16	0.45
1:D:617:ARG:HD3	1:D:617:ARG:HA	1.76	0.45
1:D:881:PRO:O	1:D:884:THR:OG1	2.18	0.45
1:B:565:ILE:HG23	1:B:566:VAL:N	2.28	0.45
1:B:698:MET:HE3	1:B:698:MET:HB2	1.86	0.45
1:C:587:TYR:HE2	1:C:600:ARG:HD2	1.82	0.45
1:C:652:TYR:HB2	1:C:696:LEU:HD21	1.99	0.45
1:B:648:THR:HG22	1:B:695:LEU:HD22	1.99	0.45
1:D:688:ASP:OD1	1:D:734:THR:OG1	2.30	0.45
1:D:766:TYR:HA	1:D:772:TYR:O	2.15	0.45
1:A:824:LYS:HA	1:A:827:LEU:HD12	1.99	0.45
1:B:867:ARG:HB3	1:B:872:MET:HE1	1.99	0.45
1:C:931:ARG:O	1:C:935:SER:HB3	2.16	0.45
1:A:688:ASP:OD1	1:A:734:THR:OG1	2.23	0.45
1:B:569:ILE:HD11	1:B:632:GLU:HB2	1.99	0.45
1:C:775:PHE:O	1:C:781:ARG:HA	2.17	0.45
1:D:649:LEU:HD23	1:D:649:LEU:HA	1.75	0.45
1:D:907:LYS:HD2	1:D:907:LYS:HA	1.78	0.45
1:B:867:ARG:NE	1:B:872:MET:HE1	2.32	0.45
1:A:839:LEU:HB2	1:A:930:VAL:HB	1.99	0.45
1:B:742:MET:SD	1:B:751:PRO:HB3	2.57	0.45
1:A:777:LYS:H	1:A:777:LYS:HG2	1.55	0.44
1:A:869:VAL:HG11	1:A:943:HIS:ND1	2.32	0.44
1:B:757:ILE:HG21	1:B:820:ARG:HB3	1.98	0.44
1:C:835:LEU:H	1:C:835:LEU:HD12	1.82	0.44
1:D:717:LYS:O	1:D:718:LEU:HD12	2.18	0.44
1:D:875:ARG:HG2	1:D:883:GLN:NE2	2.32	0.44
1:D:890:ARG:HH11	1:D:892:TYR:HD2	1.66	0.44
1:B:924:SER:N	1:B:928:ASP:HB2	2.32	0.44
1:C:690:LYS:HZ1	1:C:734:THR:HG21	1.82	0.44
1:A:905:ARG:NH1	1:A:906:ASN:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:GLN:HA	1:B:617:ARG:HE	1.83	0.44
1:C:760:ALA:HA	1:C:763:VAL:HG13	2.00	0.44
1:C:765:TYR:CD2	1:C:774:PRO:HG3	2.53	0.44
1:A:660:HIS:O	1:A:705:ILE:HD12	2.18	0.44
1:A:757:ILE:HD11	1:A:823:ALA:HA	1.99	0.44
1:D:839:LEU:HD22	1:D:842:PHE:CE2	2.53	0.44
1:B:807:GLU:OE1	1:B:811:LYS:NZ	2.31	0.44
1:D:774:PRO:HB2	1:D:775:PHE:CD1	2.53	0.44
1:D:849:ILE:HG21	1:D:898:ARG:NE	2.27	0.44
1:A:782:GLN:HA	1:A:785:ILE:HD12	1.98	0.44
1:B:649:LEU:O	1:B:653:VAL:HG23	2.17	0.44
1:D:634:ASP:HB2	1:D:639:TYR:CE1	2.49	0.44
1:A:814:ALA:O	1:A:820:ARG:NH1	2.51	0.44
1:B:564:VAL:HG12	1:B:565:ILE:N	2.32	0.44
1:B:624:ASN:O	1:B:709:ILE:HD13	2.17	0.44
1:B:817:PRO:HA	1:B:820:ARG:HG3	2.00	0.44
1:B:869:VAL:HG23	1:B:939:HIS:HB2	1.99	0.44
1:C:777:LYS:O	1:C:781:ARG:HG3	2.18	0.44
1:C:786:LEU:HD23	1:C:786:LEU:HA	1.85	0.44
1:D:679:LEU:O	1:D:684:ILE:HG23	2.18	0.44
1:D:775:PHE:N	1:D:776:GLY:HA2	2.32	0.44
1:B:564:VAL:HG21	1:B:571:PHE:CE1	2.53	0.43
1:C:781:ARG:O	1:C:785:ILE:HG13	2.17	0.43
1:A:585:ILE:HG13	1:A:586:VAL:N	2.32	0.43
1:A:608:PHE:CE1	1:A:613:VAL:HG21	2.53	0.43
1:C:824:LYS:HE2	1:C:824:LYS:HB3	1.69	0.43
1:A:633:LYS:HD2	1:A:637:PHE:O	2.18	0.43
1:B:952:ARG:HG2	1:B:961:TYR:HB3	2.01	0.43
1:A:658:PHE:CE1	1:A:660:HIS:HA	2.54	0.43
1:A:663:LEU:HD21	1:A:668:LEU:HD22	2.00	0.43
1:B:738:ILE:HG22	1:B:739:ALA:O	2.19	0.43
1:B:929:PHE:O	1:B:932:TYR:HB3	2.19	0.43
1:A:643:GLU:N	1:A:643:GLU:CD	2.76	0.43
1:B:757:ILE:HG12	1:B:821:PRO:O	2.18	0.43
1:B:761:GLY:O	1:B:764:PHE:HB2	2.19	0.43
1:A:870:VAL:HG23	1:A:897:VAL:HG22	2.00	0.43
1:C:616:LEU:CD2	1:C:712:PHE:HE2	2.31	0.43
1:C:652:TYR:HE1	1:C:660:HIS:HB3	1.83	0.43
1:A:624:ASN:ND2	1:A:671:GLN:HB3	2.34	0.43
1:A:673:THR:HG22	1:A:827:LEU:HG	2.00	0.43
1:B:845:VAL:HG22	1:B:948:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:577:LEU:N	1:D:586:VAL:O	2.35	0.43
1:D:875:ARG:NH2	1:D:892:TYR:O	2.52	0.43
1:A:732:PRO:HG2	1:A:742:MET:HE3	2.01	0.43
1:D:622:HIS:ND1	1:D:675:GLY:HA2	2.34	0.43
1:D:795:PHE:HB3	1:D:806:ARG:CG	2.48	0.43
1:D:879:THR:HG23	1:D:932:TYR:HE1	1.84	0.43
1:B:627:ARG:H	1:B:643:GLU:CD	2.26	0.43
1:C:886:LEU:HD12	1:C:892:TYR:HD2	1.84	0.43
1:A:665:PRO:O	1:A:668:LEU:HB3	2.19	0.42
1:A:882:LEU:HD22	1:A:886:LEU:HD22	2.01	0.42
1:B:571:PHE:HE2	1:B:639:TYR:HE2	1.67	0.42
1:B:736:GLY:O	1:B:773:HIS:CE1	2.72	0.42
1:C:740:PRO:HG3	1:C:815:MET:HG2	2.01	0.42
1:A:924:SER:O	1:A:925:ILE:HB	2.18	0.42
1:B:874:TRP:HB2	1:B:937:PHE:CZ	2.54	0.42
1:D:633:LYS:HD2	1:D:638:GLN:HG3	2.02	0.42
1:B:686:HIS:O	1:B:687:ARG:HB2	2.19	0.42
1:C:754:THR:HB	1:C:820:ARG:HE	1.84	0.42
1:D:816:ASP:HA	1:D:817:PRO:HD2	1.88	0.42
1:D:960:TYR:N	1:D:960:TYR:CD1	2.88	0.42
1:B:607:SER:OG	1:B:715:CYS:SG	2.78	0.42
1:B:740:PRO:CD	1:B:785:ILE:HD11	2.49	0.42
1:B:777:LYS:HA	1:B:777:LYS:HD3	1.41	0.42
1:A:698:MET:HE3	1:A:698:MET:HB2	1.84	0.42
1:C:663:LEU:C	1:C:663:LEU:HD12	2.44	0.42
1:D:622:HIS:CE1	1:D:675:GLY:HA2	2.54	0.42
1:D:837:LYS:HE3	1:D:837:LYS:HB3	1.62	0.42
1:D:839:LEU:HD23	1:D:930:VAL:CG1	2.50	0.42
1:C:586:VAL:CG1	1:C:599:LYS:HB3	2.48	0.42
1:C:773:HIS:HB3	1:C:776:GLY:O	2.20	0.42
1:C:835:LEU:HD22	1:C:927:ASP:HA	2.00	0.42
1:D:600:ARG:HG3	1:D:637:PHE:HE2	1.84	0.42
1:A:584:THR:HG23	1:A:601:ILE:HG22	2.02	0.42
1:B:572:CYS:HA	1:B:573:PRO:HD3	1.86	0.42
1:D:600:ARG:HG3	1:D:637:PHE:CE2	2.55	0.42
1:A:828:LYS:HD2	1:A:962:TRP:HB2	2.01	0.42
1:A:858:ILE:HD11	1:A:951:CYS:SG	2.60	0.42
1:D:664:GLU:O	1:D:667:THR:OG1	2.26	0.42
1:D:665:PRO:O	1:D:668:LEU:HB3	2.19	0.42
1:B:697:SER:O	1:B:705:ILE:HD12	2.20	0.42
1:C:712:PHE:CD1	1:C:712:PHE:N	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:ARG:NH2	1:C:810:GLU:OE2	2.51	0.42
1:D:681:SER:OG	1:D:682:LEU:HD12	2.20	0.42
1:D:948:MET:HB3	1:D:948:MET:HE2	1.59	0.42
1:A:568:LYS:NZ	1:A:630:CYS:HB2	2.34	0.41
1:A:696:LEU:HD12	1:A:707:ALA:HA	2.01	0.41
1:B:829:HIS:CG	1:B:830:PRO:HD2	2.55	0.41
1:C:626:ILE:HG22	1:C:712:PHE:HE1	1.84	0.41
1:D:743:LEU:CD2	1:D:786:LEU:HD11	2.50	0.41
1:C:768:ILE:C	1:C:770:GLU:H	2.29	0.41
1:D:764:PHE:HB3	1:D:809:ILE:CD1	2.50	0.41
1:D:941:LEU:HD13	1:D:941:LEU:C	2.45	0.41
1:A:732:PRO:HG2	1:A:742:MET:CE	2.50	0.41
1:C:869:VAL:HG23	1:C:939:HIS:CB	2.50	0.41
1:C:829:HIS:CG	1:C:830:PRO:HD2	2.54	0.41
1:C:842:PHE:CZ	1:C:941:LEU:HD22	2.56	0.41
1:D:628:TYR:CD1	1:D:640:ILE:HD11	2.55	0.41
1:A:664:GLU:HB2	1:A:667:THR:HG23	2.02	0.41
1:B:680:HIS:NE2	1:B:753:TYR:HB2	2.33	0.41
1:C:867:ARG:NH1	1:D:806:ARG:HE	2.18	0.41
1:D:914:LEU:HD12	1:D:914:LEU:N	2.36	0.41
1:A:624:ASN:ND2	1:A:707:ALA:O	2.40	0.41
1:B:758:PHE:HB2	1:B:820:ARG:NE	2.34	0.41
1:C:652:TYR:CE1	1:C:660:HIS:HB3	2.56	0.41
1:D:801:GLU:H	1:D:801:GLU:CD	2.29	0.41
1:D:834:SER:H	1:D:837:LYS:CE	2.34	0.41
1:C:872:MET:HE2	1:D:806:ARG:HD3	2.02	0.41
1:A:626:ILE:HG12	1:A:643:GLU:OE1	2.21	0.41
1:B:736:GLY:O	1:B:773:HIS:HE1	2.03	0.41
1:B:759:SER:O	1:B:763:VAL:HG12	2.21	0.41
1:B:821:PRO:HG2	1:B:826:VAL:HG22	2.03	0.41
1:D:960:TYR:N	1:D:960:TYR:HD1	2.18	0.41
1:A:568:LYS:HE3	1:A:591:PHE:CE1	2.39	0.41
1:A:918:VAL:HG23	1:A:922:LEU:HD22	2.03	0.41
1:C:799:LYS:HE2	1:C:799:LYS:HB3	1.74	0.41
1:D:591:PHE:HB3	1:D:592:ASP:H	1.70	0.41
1:D:592:ASP:OD1	1:D:593:ASN:N	2.46	0.41
1:D:706:LYS:HG2	1:D:707:ALA:N	2.35	0.41
1:D:738:ILE:HG22	1:D:739:ALA:O	2.21	0.41
1:D:759:SER:O	1:D:763:VAL:HG12	2.20	0.41
1:B:646:ALA:HB2	1:B:698:MET:HG2	2.03	0.41
1:B:764:PHE:HB3	1:B:809:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:800:HIS:HD2	1:D:941:LEU:HD12	1.86	0.41
1:D:839:LEU:HD22	1:D:839:LEU:HA	1.78	0.41
1:A:757:ILE:HD13	1:A:757:ILE:HA	1.97	0.40
1:B:614:GLN:HA	1:B:617:ARG:NE	2.37	0.40
1:C:600:ARG:HG3	1:C:637:PHE:HE2	1.85	0.40
1:A:647:ALA:HB1	1:A:651:GLU:HB2	2.03	0.40
1:C:611:ARG:H	1:C:611:ARG:HG2	1.67	0.40
1:C:616:LEU:HD11	1:C:684:ILE:HD13	2.03	0.40
1:D:841:PHE:CE2	1:D:960:TYR:HA	2.56	0.40
1:A:594:ARG:HH11	1:B:593:ASN:HB2	1.86	0.40
1:B:565:ILE:HD12	1:B:565:ILE:HA	1.76	0.40
1:B:565:ILE:CG2	1:B:566:VAL:H	2.31	0.40
1:B:886:LEU:HD12	1:B:907:LYS:HE3	2.04	0.40
1:C:867:ARG:CZ	1:C:872:MET:HE3	2.52	0.40
1:C:869:VAL:HG11	1:C:943:HIS:ND1	2.37	0.40
1:D:686:HIS:ND1	1:D:712:PHE:HB3	2.36	0.40
1:D:795:PHE:HE2	1:D:809:ILE:HG13	1.86	0.40
1:B:737:TRP:O	1:B:759:SER:OG	2.29	0.40
1:B:867:ARG:CZ	1:B:872:MET:HE1	2.51	0.40
1:C:874:TRP:CD2	1:C:900:LEU:HD13	2.56	0.40
1:C:566:VAL:O	1:C:566:VAL:HG22	2.22	0.40
1:C:690:LYS:HG3	1:C:692:HIS:H	1.86	0.40
1:C:741:GLU:CD	1:C:820:ARG:HH22	2.29	0.40
1:C:846:SER:OG	1:C:902:ARG:HA	2.22	0.40
1:C:881:PRO:HG2	1:C:921:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	379/435 (87%)	332 (88%)	39 (10%)	8 (2%)	5 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	378/435 (87%)	333 (88%)	35 (9%)	10 (3%)	4	23
1	C	378/435 (87%)	344 (91%)	30 (8%)	4 (1%)	11	43
1	D	367/435 (84%)	323 (88%)	39 (11%)	5 (1%)	9	36
All	All	1502/1740 (86%)	1332 (89%)	143 (10%)	27 (2%)	6	31

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	893	LYS
1	A	924	SER
1	C	925	ILE
1	D	889	PHE
1	A	593	ASN
1	A	644	LEU
1	B	567	GLY
1	C	866	GLY
1	B	831	PHE
1	B	890	ARG
1	B	891	THR
1	C	867	ARG
1	A	866	GLY
1	B	565	ILE
1	B	923	GLY
1	B	925	ILE
1	D	593	ASN
1	D	659	ALA
1	D	925	ILE
1	A	629	PHE
1	A	925	ILE
1	B	867	ARG
1	A	872	MET
1	B	866	GLY
1	D	776	GLY
1	C	566	VAL
1	B	776	GLY

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	330/387 (85%)	281 (85%)	49 (15%)	3	15
1	B	335/387 (87%)	285 (85%)	50 (15%)	3	15
1	C	336/387 (87%)	292 (87%)	44 (13%)	4	19
1	D	327/387 (84%)	277 (85%)	50 (15%)	3	14
All	All	1328/1548 (86%)	1135 (86%)	193 (14%)	3	15

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	564	VAL
1	A	568	LYS
1	A	585	ILE
1	A	602	LEU
1	A	620	ASP
1	A	625	VAL
1	A	627	ARG
1	A	636	GLN
1	A	640	ILE
1	A	642	ILE
1	A	648	THR
1	A	658	PHE
1	A	668	LEU
1	A	673	THR
1	A	676	LEU
1	A	679	LEU
1	A	684	ILE
1	A	696	LEU
1	A	702	HIS
1	A	705	ILE
1	A	709	ILE
1	A	711	ASP
1	A	738	ILE
1	A	743	LEU
1	A	755	VAL
1	A	763	VAL
1	A	777	LYS
1	A	787	LEU
1	A	792	LEU
1	A	809	ILE

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Mol	Chain	Res	Type
1	A	819	GLN
1	A	827	LEU
1	A	843	GLN
1	A	852	GLU
1	A	869	VAL
1	A	878	ILE
1	A	879	THR
1	A	880	VAL
1	A	882	LEU
1	A	886	LEU
1	A	891	THR
1	A	914	LEU
1	A	918	VAL
1	A	921	THR
1	A	922	LEU
1	A	935	SER
1	A	941	LEU
1	A	956	LEU
1	A	959	THR
1	B	566	VAL
1	B	568	LYS
1	B	569	ILE
1	B	586	VAL
1	B	596	VAL
1	B	620	ASP
1	B	626	ILE
1	B	636	GLN
1	B	642	ILE
1	B	644	LEU
1	B	650	GLN
1	B	660	HIS
1	B	661	LEU
1	B	668	LEU
1	B	673	THR
1	B	676	LEU
1	B	684	ILE
1	B	702	HIS
1	B	709	ILE
1	B	711	ASP
1	B	718	LEU
1	B	731	VAL
1	B	757	ILE

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Mol	Chain	Res	Type
1	B	763	VAL
1	B	777	LYS
1	B	785	ILE
1	B	809	ILE
1	B	815	MET
1	B	819	GLN
1	B	820	ARG
1	B	824	LYS
1	B	827	LEU
1	B	834	SER
1	B	850	GLU
1	B	854	LEU
1	B	858	ILE
1	B	878	ILE
1	B	879	THR
1	B	880	VAL
1	B	882	LEU
1	B	884	THR
1	B	886	LEU
1	B	893	LYS
1	B	904	MET
1	B	916	VAL
1	B	920	GLU
1	B	921	THR
1	B	922	LEU
1	B	941	LEU
1	B	952	ARG
1	C	568	LYS
1	C	582	GLU
1	C	586	VAL
1	C	602	LEU
1	C	627	ARG
1	C	636	GLN
1	C	640	ILE
1	C	642	ILE
1	C	649	LEU
1	C	663	LEU
1	C	668	LEU
1	C	676	LEU
1	C	679	LEU
1	C	684	ILE
1	C	696	LEU

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Mol	Chain	Res	Type
1	C	702	HIS
1	C	709	ILE
1	C	710	SER
1	C	712	PHE
1	C	716	LYS
1	C	738	ILE
1	C	742	MET
1	C	743	LEU
1	C	763	VAL
1	C	790	CYS
1	C	822	SER
1	C	828	LYS
1	C	849	ILE
1	C	852	GLU
1	C	863	GLU
1	C	870	VAL
1	C	878	ILE
1	C	880	VAL
1	C	882	LEU
1	C	893	LYS
1	C	906	ASN
1	C	916	VAL
1	C	918	VAL
1	C	930	VAL
1	C	935	SER
1	C	941	LEU
1	C	952	ARG
1	C	953	HIS
1	C	956	LEU
1	D	577	LEU
1	D	582	GLU
1	D	598	VAL
1	D	600	ARG
1	D	611	ARG
1	D	617	ARG
1	D	651	GLU
1	D	656	LYS
1	D	661	LEU
1	D	668	LEU
1	D	673	THR
1	D	676	LEU
1	D	684	ILE

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Mol	Chain	Res	Type
1	D	685	VAL
1	D	689	LEU
1	D	702	HIS
1	D	716	LYS
1	D	743	LEU
1	D	763	VAL
1	D	767	VAL
1	D	770	GLU
1	D	792	LEU
1	D	807	GLU
1	D	819	GLN
1	D	820	ARG
1	D	825	HIS
1	D	837	LYS
1	D	839	LEU
1	D	843	GLN
1	D	845	VAL
1	D	855	ASP
1	D	859	VAL
1	D	860	ARG
1	D	870	VAL
1	D	878	ILE
1	D	880	VAL
1	D	886	LEU
1	D	893	LYS
1	D	907	LYS
1	D	914	LEU
1	D	920	GLU
1	D	929	PHE
1	D	930	VAL
1	D	940	LEU
1	D	941	LEU
1	D	944	THR
1	D	948	MET
1	D	949	GLU
1	D	959	THR
1	D	960	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	692	HIS

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Mol	Chain	Res	Type
1	A	939	HIS
1	A	953	HIS
1	B	624	ASN
1	B	773	HIS
1	C	614	GLN
1	C	700	ASN
1	C	800	HIS
1	C	861	GLN
1	C	910	HIS
1	D	614	GLN
1	D	622	HIS
1	D	671	GLN
1	D	686	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	D	1001	5	28,29,29	1.53	5 (17%)	43,45,45	1.78	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	1002	5	28,29,29	1.43	5 (17%)	43,45,45	1.84	11 (25%)
3	ADP	B	1001	5	28,29,29	1.53	5 (17%)	43,45,45	1.66	9 (20%)
4	PEU	A	1003	-	18,18,82	0.65	0	17,17,81	1.67	2 (11%)
2	31K	A	1001	1	23,23,23	0.83	1 (4%)	29,33,33	2.17	9 (31%)
3	ADP	C	1001	5	28,29,29	1.51	5 (17%)	43,45,45	1.65	8 (18%)

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	D	1001	5	-	9/16/32/32	0/3/3/3
3	ADP	A	1002	5	-	3/16/32/32	0/3/3/3
3	ADP	B	1001	5	-	2/16/32/32	0/3/3/3
4	PEU	A	1003	-	-	7/16/16/80	-
2	31K	A	1001	1	-	2/6/16/16	0/3/3/3
3	ADP	C	1001	5	-	1/16/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	ADP	C5-C4	5.41	1.48	1.39
3	D	1001	ADP	C5-C4	5.28	1.48	1.39
3	C	1001	ADP	C5-C4	5.12	1.48	1.39
3	A	1002	ADP	C5-C4	5.04	1.48	1.39
3	B	1001	ADP	C8-N7	2.87	1.37	1.31
3	C	1001	ADP	C8-N7	2.85	1.37	1.31
3	D	1001	ADP	C8-N7	2.70	1.36	1.31
3	D	1001	ADP	C5-C6	2.70	1.48	1.41
3	B	1001	ADP	C5-C6	2.64	1.48	1.41
3	C	1001	ADP	C5-N7	-2.59	1.34	1.39
3	A	1002	ADP	C8-N7	2.53	1.36	1.31
3	A	1002	ADP	C5-C6	2.35	1.47	1.41
2	A	1001	31K	C11-C03	2.33	1.42	1.39
3	D	1001	ADP	PA-O3A	2.25	1.61	1.59
3	C	1001	ADP	C5-C6	2.16	1.47	1.41
3	D	1001	ADP	C5-N7	-2.13	1.35	1.39
3	B	1001	ADP	C4-N9	-2.12	1.33	1.37
3	C	1001	ADP	C4-N9	-2.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	ADP	C5-N7	-2.09	1.35	1.39
3	A	1002	ADP	C4-N9	-2.06	1.33	1.37
3	B	1001	ADP	PA-O3A	2.00	1.61	1.59

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	31K	O07-C06-C04	6.77	121.62	114.53
3	D	1001	ADP	C5-C4-N3	-5.47	119.19	126.72
3	C	1001	ADP	C5-C4-N3	-4.90	119.97	126.72
3	B	1001	ADP	C5-C4-N3	-4.78	120.13	126.72
3	D	1001	ADP	N3-C4-N9	4.46	134.75	127.17
3	A	1002	ADP	C5-C4-N3	-4.30	120.79	126.72
3	C	1001	ADP	N3-C4-N9	4.20	134.31	127.17
3	A	1002	ADP	N3-C4-N9	4.11	134.16	127.17
2	A	1001	31K	C19-O20-C21	4.02	120.75	113.67
3	B	1001	ADP	N3-C4-N9	3.93	133.84	127.17
3	A	1002	ADP	N3-C2-N1	-3.65	123.06	128.58
3	D	1001	ADP	C2-N3-C4	3.62	120.67	111.83
3	D	1001	ADP	N3-C2-N1	-3.52	123.25	128.58
3	A	1002	ADP	C4-N9-C8	3.38	109.28	105.74
3	C	1001	ADP	N3-C2-N1	-3.29	123.60	128.58
3	B	1001	ADP	C2-N3-C4	3.22	119.70	111.83
3	C	1001	ADP	C2-N3-C4	3.21	119.68	111.83
3	B	1001	ADP	N3-C2-N1	-3.18	123.76	128.58
3	A	1002	ADP	C2-N3-C4	3.14	119.50	111.83
2	A	1001	31K	C08-O07-C06	3.14	122.11	117.51
2	A	1001	31K	O20-C21-C22	3.09	121.81	117.12
2	A	1001	31K	C09-C10-C12	-2.99	115.83	120.84
2	A	1001	31K	O07-C06-C09	-2.87	119.13	124.08
3	D	1001	ADP	C4-C5-N7	-2.81	107.37	110.58
3	A	1002	ADP	C2-N1-C6	2.64	123.07	118.73
3	A	1002	ADP	C2'-C1'-N9	-2.64	106.75	113.30
3	C	1001	ADP	C3'-C2'-C1'	2.52	106.22	101.46
3	A	1002	ADP	O3B-PB-O2B	2.47	117.07	107.80
2	A	1001	31K	O20-C21-C15	-2.43	117.46	122.07
3	D	1001	ADP	O3A-PA-O1A	-2.40	103.47	110.70
3	B	1001	ADP	O3B-PB-O2B	2.38	116.74	107.80
3	B	1001	ADP	C4-C5-N7	-2.37	107.87	110.58
3	B	1001	ADP	C4-N9-C8	2.33	108.19	105.74
3	D	1001	ADP	C4-N9-C8	2.27	108.12	105.74
3	A	1002	ADP	C3'-C2'-C1'	2.23	105.69	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	ADP	N6-C6-N1	2.22	123.33	118.38
3	B	1001	ADP	C3'-C2'-C1'	2.22	105.66	101.46
2	A	1001	31K	C11-C10-C12	2.21	124.55	120.84
3	D	1001	ADP	C3'-C2'-C1'	2.19	105.61	101.46
4	A	1003	PEU	OBV-CBU-CBT	2.19	120.34	110.35
3	D	1001	ADP	C2-N1-C6	2.14	122.25	118.73
3	C	1001	ADP	C2-N1-C6	2.12	122.22	118.73
3	C	1001	ADP	C4-N9-C8	2.12	107.97	105.74
2	A	1001	31K	C13-C12-C10	-2.11	117.61	121.25
3	B	1001	ADP	C2-N1-C6	2.11	122.19	118.73
3	A	1002	ADP	C4-C5-N7	-2.09	108.20	110.58
3	C	1001	ADP	N6-C6-N1	2.07	122.98	118.38
4	A	1003	PEU	OBV-CBZ-CCA	2.06	119.17	110.11

There are no chirality outliers.

All (24) torsion outliers are listed below:

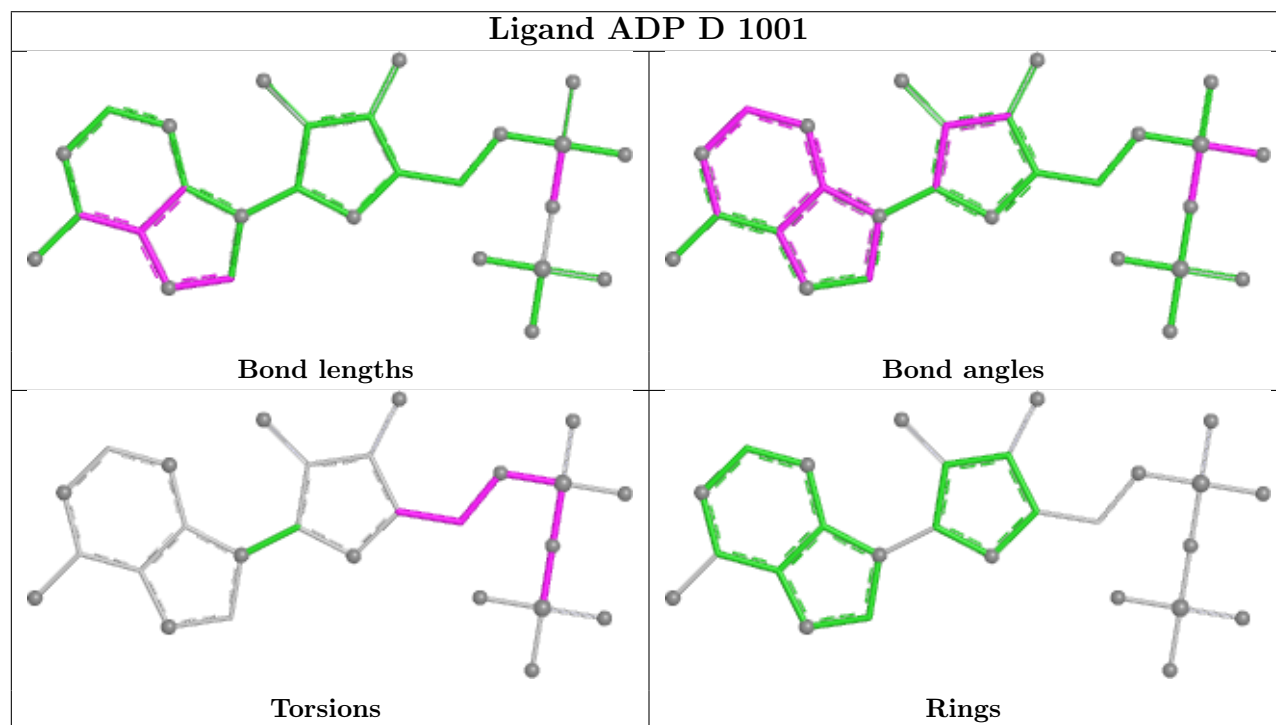
Mol	Chain	Res	Type	Atoms
3	D	1001	ADP	PA-O3A-PB-O2B
3	D	1001	ADP	PA-O3A-PB-O3B
3	D	1001	ADP	C5'-O5'-PA-O1A
3	D	1001	ADP	C5'-O5'-PA-O2A
4	A	1003	PEU	CBN-CBO-OBP-CBQ
2	A	1001	31K	C04-C06-O07-C08
4	A	1003	PEU	OBV-CBW-CBX-OBV
2	A	1001	31K	C09-C06-O07-C08
4	A	1003	PEU	OBM-CBN-CBO-OBP
4	A	1003	PEU	OBP-CBQ-CBR-OBS
4	A	1003	PEU	OBS-CBT-CBU-OBV
3	B	1001	ADP	PB-O3A-PA-O5'
4	A	1003	PEU	CBT-CBU-OBV-CBW
4	A	1003	PEU	OBV-CBZ-CCA-OCB
3	C	1001	ADP	C5'-O5'-PA-O1A
3	D	1001	ADP	C5'-O5'-PA-O3A
3	A	1002	ADP	PA-O3A-PB-O1B
3	B	1001	ADP	PA-O3A-PB-O1B
3	D	1001	ADP	C4'-C5'-O5'-PA
3	A	1002	ADP	PA-O3A-PB-O2B
3	A	1002	ADP	PA-O3A-PB-O3B
3	D	1001	ADP	PB-O3A-PA-O1A
3	D	1001	ADP	PB-O3A-PA-O2A
3	D	1001	ADP	O4'-C4'-C5'-O5'

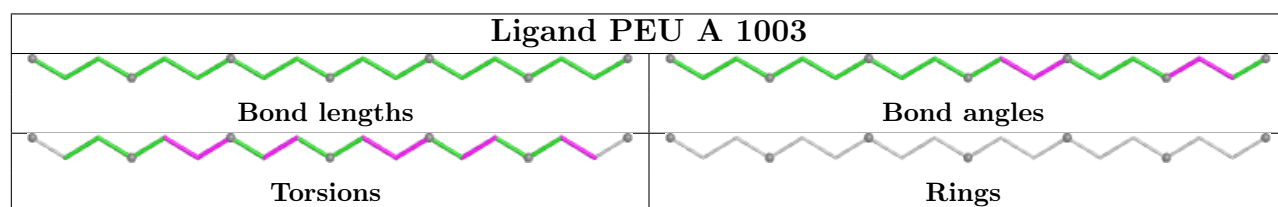
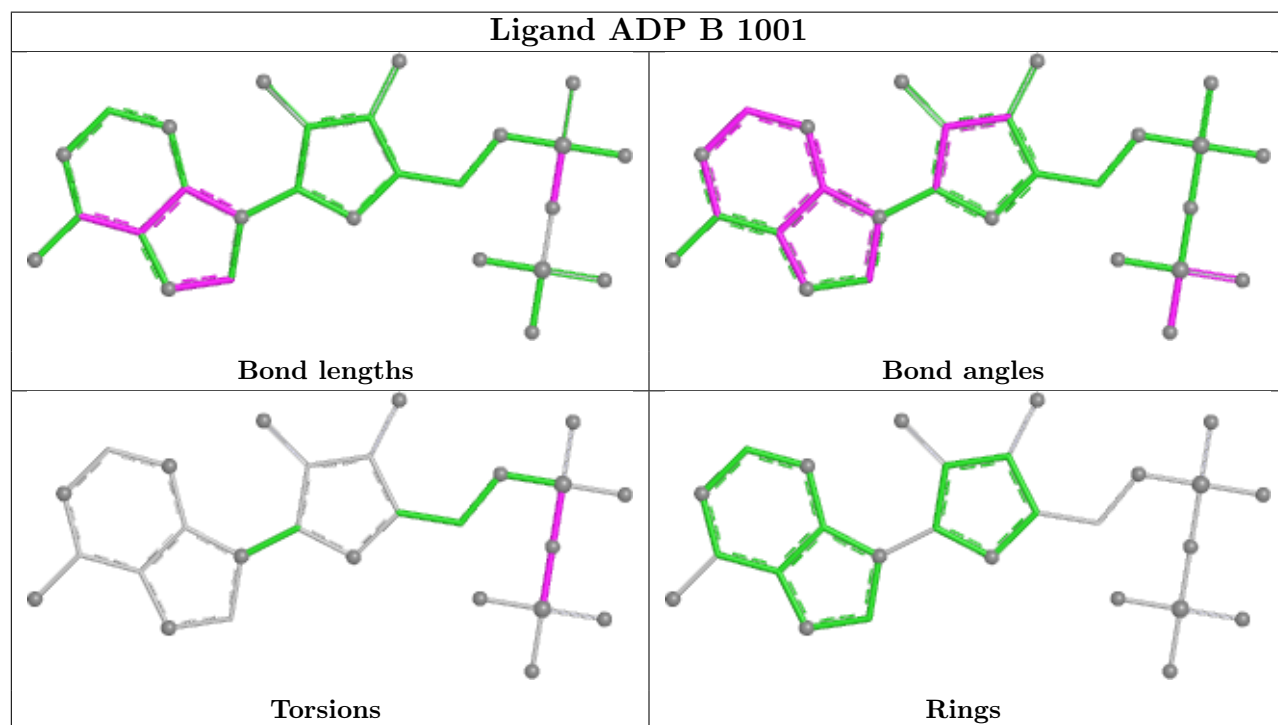
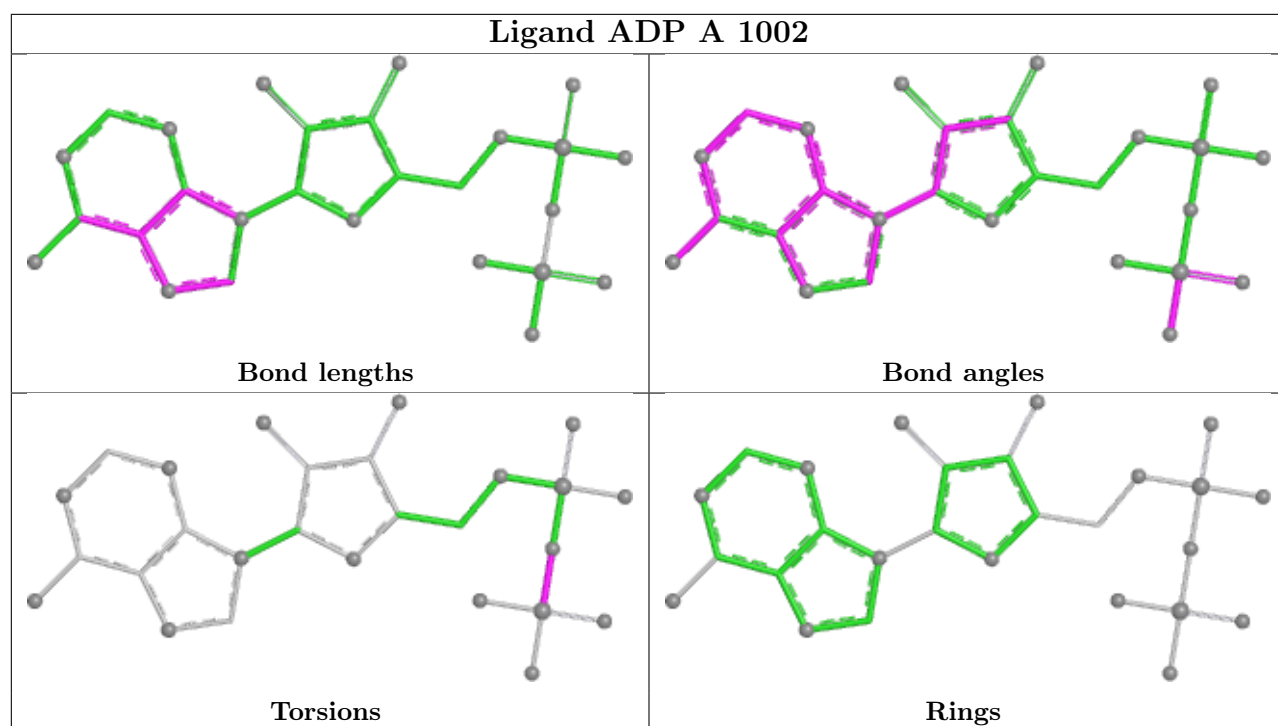
There are no ring outliers.

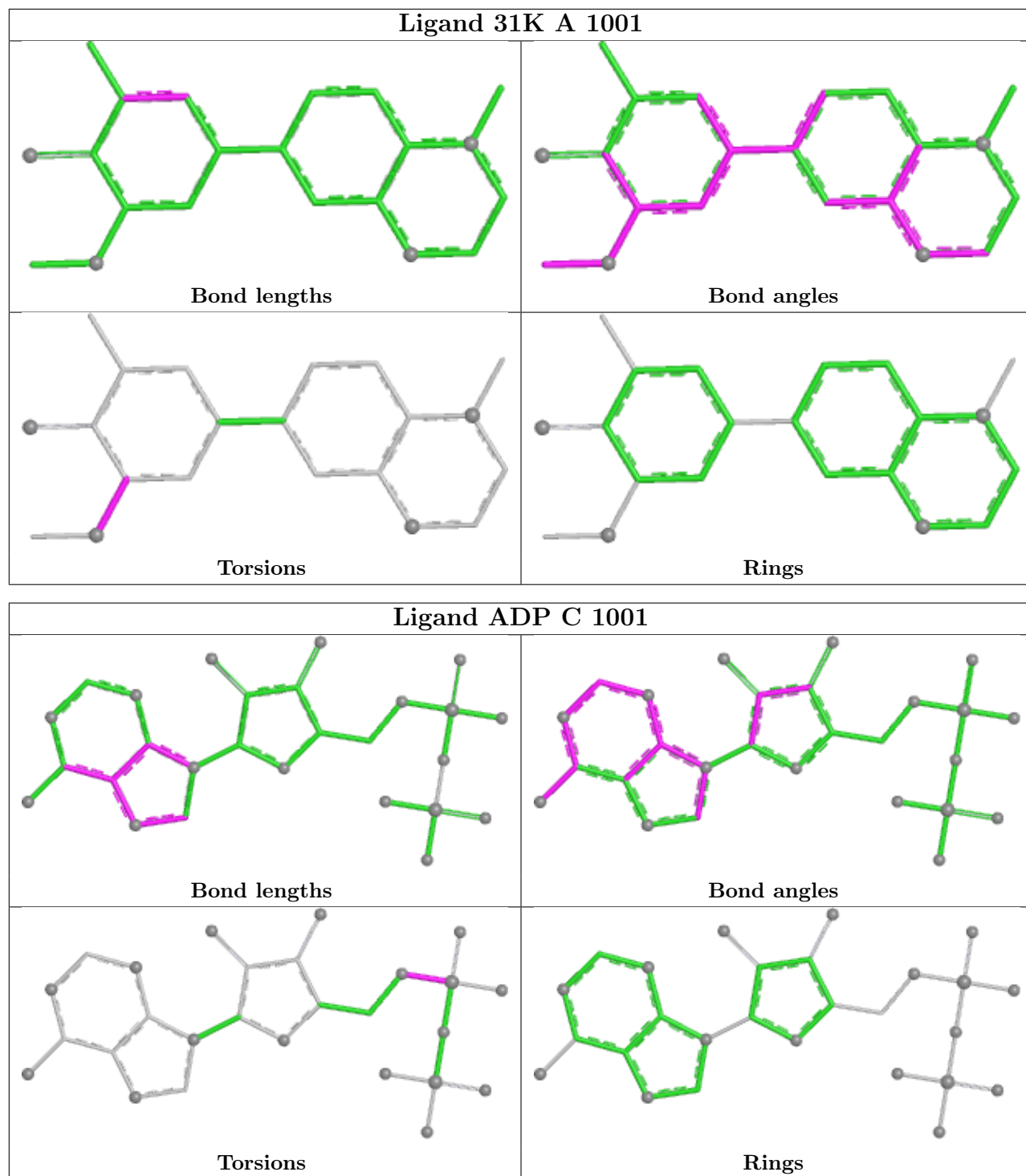
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	ADP	1	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 ⓘ

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	385/435 (88%)	0.17	20 (5%) 33 17	26, 72, 123, 181	0
1	B	384/435 (88%)	0.05	7 (1%) 67 44	33, 72, 114, 144	0
1	C	384/435 (88%)	0.11	11 (2%) 53 31	37, 78, 120, 179	0
1	D	377/435 (86%)	0.80	23 (6%) 27 14	60, 112, 161, 210	0
All	All	1530/1740 (87%)	0.28	61 (3%) 42 23	26, 84, 144, 210	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	838	GLN	4.7
1	A	593	ASN	4.6
1	D	715	CYS	4.3
1	A	567	GLY	4.2
1	D	661	LEU	4.1
1	D	842	PHE	3.6
1	A	660	HIS	3.5
1	A	661	LEU	3.3
1	C	963	HIS	3.1
1	D	751	PRO	3.1
1	A	632	GLU	3.1
1	C	962	TRP	3.0
1	D	903	ALA	2.9
1	D	929	PHE	2.8
1	D	885	ASP	2.8
1	D	892	TYR	2.8
1	A	566	VAL	2.8
1	D	880	VAL	2.8
1	D	916	VAL	2.8
1	D	771	GLY	2.8
1	A	719	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	699	PRO	2.7
1	C	889	PHE	2.7
1	A	963	HIS	2.6
1	D	926	PRO	2.6
1	D	891	THR	2.6
1	A	851	LYS	2.6
1	D	906	ASN	2.6
1	D	907	LYS	2.5
1	B	731	VAL	2.5
1	B	751	PRO	2.5
1	C	853	ALA	2.4
1	A	562	ARG	2.4
1	C	951	CYS	2.4
1	A	863	GLU	2.4
1	D	886	LEU	2.4
1	D	710	SER	2.4
1	A	858	ILE	2.3
1	C	854	LEU	2.3
1	D	919	GLN	2.3
1	A	568	LYS	2.3
1	A	569	ILE	2.3
1	B	565	ILE	2.3
1	A	872	MET	2.3
1	C	891	THR	2.3
1	D	578	GLY	2.2
1	A	629	PHE	2.2
1	C	628	TYR	2.2
1	C	645	CYS	2.1
1	B	718	LEU	2.1
1	B	819	GLN	2.1
1	D	641	ALA	2.1
1	B	562	ARG	2.1
1	A	659	ALA	2.1
1	B	597	ALA	2.1
1	A	589	GLY	2.1
1	D	905	ARG	2.1
1	D	753	TYR	2.0
1	C	566	VAL	2.0
1	A	855	ASP	2.0
1	A	616	LEU	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](#)

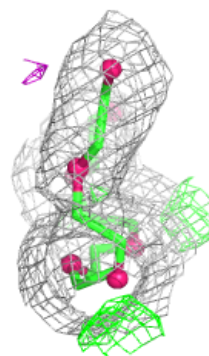
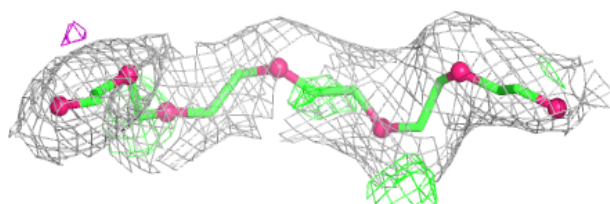
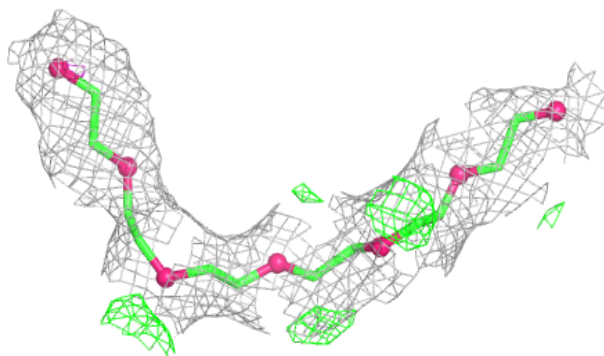
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	PEU	A	1003	19/83	0.88	0.13	28,65,98,107	0
3	ADP	D	1001	27/27	0.90	0.12	30,77,106,117	0
2	31K	A	1001	21/21	0.90	0.15	71,95,109,116	0
3	ADP	B	1001	27/27	0.94	0.09	38,54,77,180	0
5	MG	D	1002	1/1	0.94	0.07	65,65,65,65	0
5	MG	C	1002	1/1	0.95	0.12	98,98,98,98	0
3	ADP	A	1002	27/27	0.96	0.08	23,48,79,90	0
3	ADP	C	1001	27/27	0.96	0.09	34,61,86,165	0
5	MG	B	1002	1/1	0.97	0.09	53,53,53,53	0
5	MG	A	1004	1/1	0.98	0.07	42,42,42,42	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.

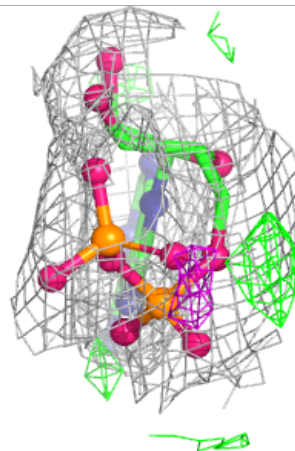
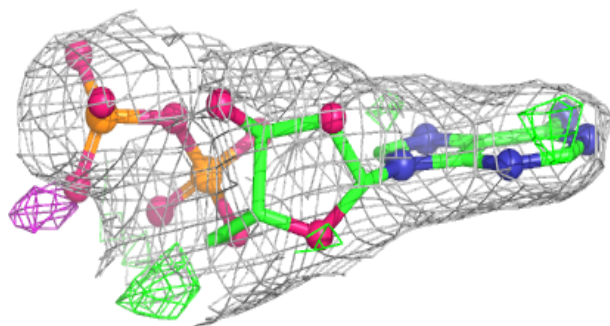
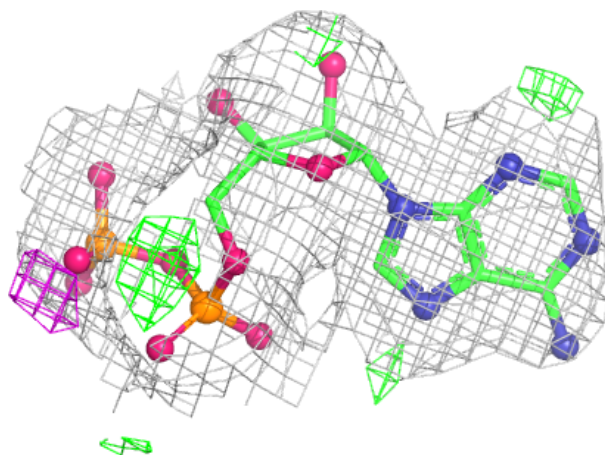
Electron density around PEU A 1003:

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



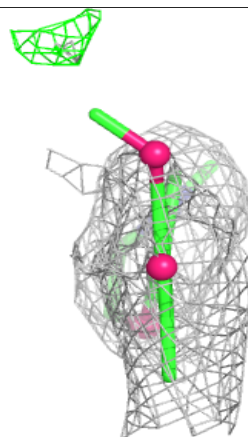
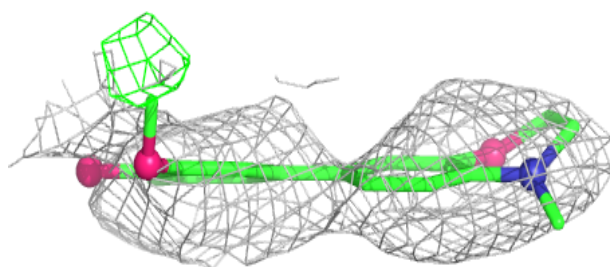
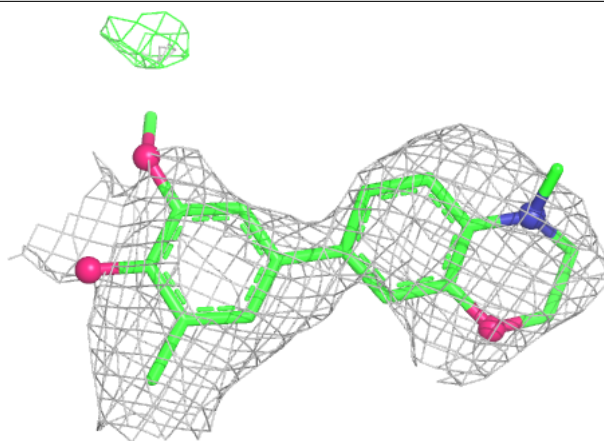
Electron density around ADP D 1001:

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



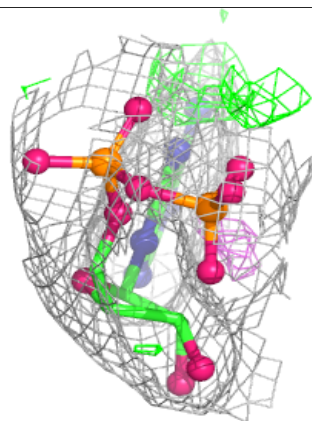
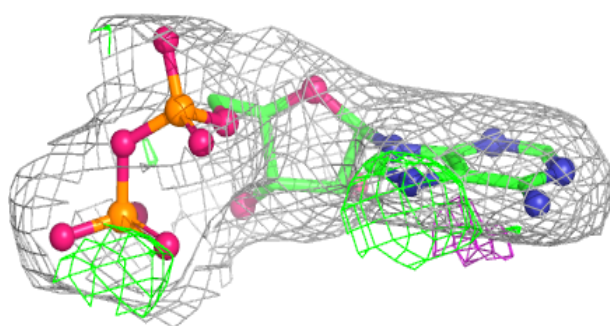
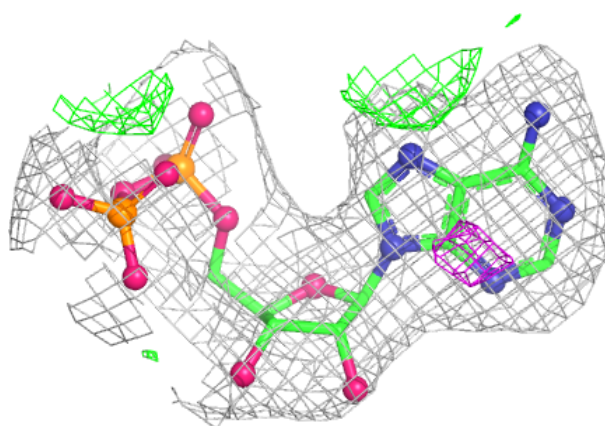
Electron density around 31K A 1001:

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

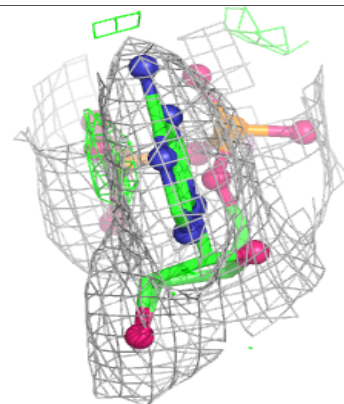
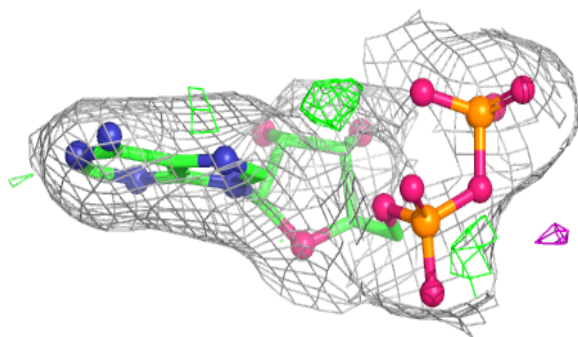
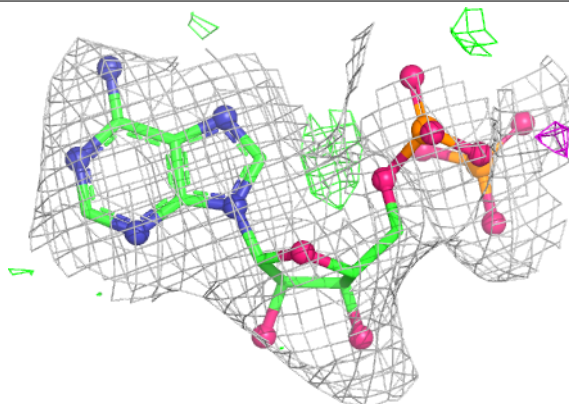


Electron density around ADP B 1001:

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

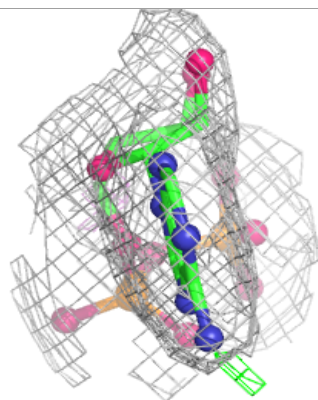
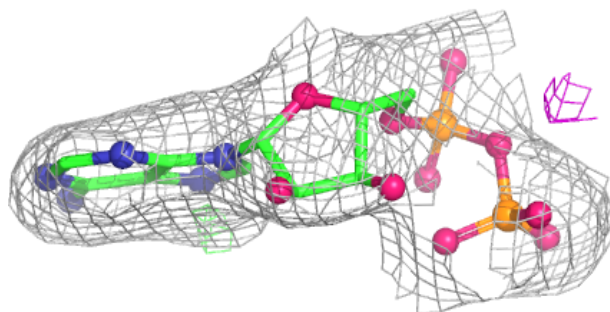
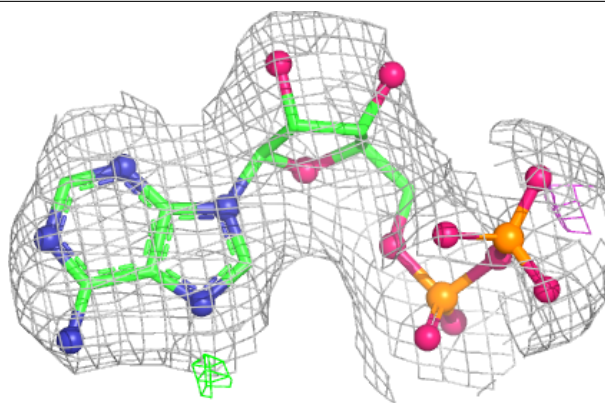
**Electron density around ADP A 1002:**

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



Electron density around ADP C 1001:

$2mF_o - DF_c$ (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.