



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 2NUU / pdb_00002nuu
Title : Regulating the Escherichia coli ammonia channel: the crystal structure of the AmtB-GlnK complex
Authors : Conroy, M.J.; Durand, A.; Lupo, D.; Li, X.-D.; Bullough, P.A.; Winkler, F.K.; Merrick, M.
Deposited on : 2006-11-09
Resolution : 2.50 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

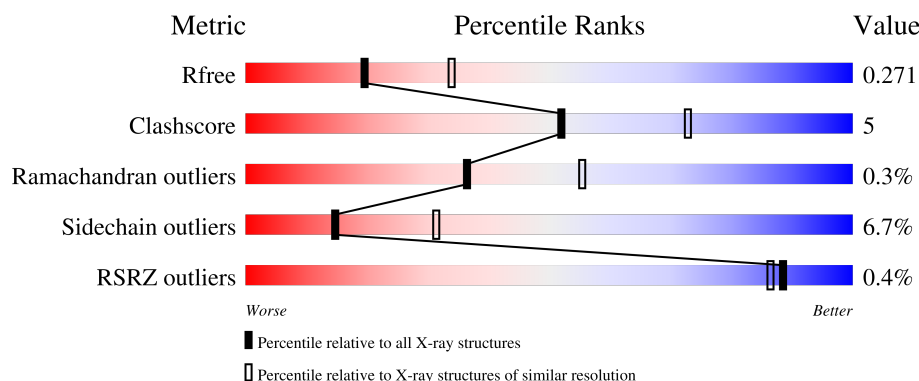
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	415	
1	B	415	
1	C	415	
1	D	415	

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Mol	Chain	Length	Quality of chain
1	E	415	 84%13%..
1	F	415	 82%16%..
2	G	112	 85%14%. .
2	H	112	 75%22%. .
2	I	112	 79%20%. .
2	J	112	 82%14%. .
2	K	112	 75%18%7%. .
2	L	112	 74%23%. .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24026 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 Ammonia channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3020	1981	501	519	19			
1	B	409	Total	C	N	O	S	0	0	0
			3020	1981	501	519	19			
1	C	409	Total	C	N	O	S	0	0	0
			3020	1981	501	519	19			
1	D	410	Total	C	N	O	S	0	0	0
			3030	1987	504	520	19			
1	E	409	Total	C	N	O	S	0	0	0
			3020	1981	501	519	19			
1	F	409	Total	C	N	O	S	0	0	0
			3020	1981	501	519	19			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	expression tag	UNP P69681
A	-7	PRO	-	expression tag	UNP P69681
A	-6	ALA	-	expression tag	UNP P69681
A	-5	VAL	-	expression tag	UNP P69681
A	-4	ALA	-	expression tag	UNP P69681
A	-3	HIS	-	expression tag	UNP P69681
A	-2	HIS	-	expression tag	UNP P69681
A	-1	HIS	-	expression tag	UNP P69681
A	0	HIS	-	expression tag	UNP P69681
A	1	HIS	-	expression tag	UNP P69681
A	2	HIS	-	expression tag	UNP P69681
B	-8	ALA	-	expression tag	UNP P69681
B	-7	PRO	-	expression tag	UNP P69681
B	-6	ALA	-	expression tag	UNP P69681
B	-5	VAL	-	expression tag	UNP P69681
B	-4	ALA	-	expression tag	UNP P69681
B	-3	HIS	-	expression tag	UNP P69681

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP P69681
B	-1	HIS	-	expression tag	UNP P69681
B	0	HIS	-	expression tag	UNP P69681
B	1	HIS	-	expression tag	UNP P69681
B	2	HIS	-	expression tag	UNP P69681
C	-8	ALA	-	expression tag	UNP P69681
C	-7	PRO	-	expression tag	UNP P69681
C	-6	ALA	-	expression tag	UNP P69681
C	-5	VAL	-	expression tag	UNP P69681
C	-4	ALA	-	expression tag	UNP P69681
C	-3	HIS	-	expression tag	UNP P69681
C	-2	HIS	-	expression tag	UNP P69681
C	-1	HIS	-	expression tag	UNP P69681
C	0	HIS	-	expression tag	UNP P69681
C	1	HIS	-	expression tag	UNP P69681
C	2	HIS	-	expression tag	UNP P69681
D	-8	ALA	-	expression tag	UNP P69681
D	-7	PRO	-	expression tag	UNP P69681
D	-6	ALA	-	expression tag	UNP P69681
D	-5	VAL	-	expression tag	UNP P69681
D	-4	ALA	-	expression tag	UNP P69681
D	-3	HIS	-	expression tag	UNP P69681
D	-2	HIS	-	expression tag	UNP P69681
D	-1	HIS	-	expression tag	UNP P69681
D	0	HIS	-	expression tag	UNP P69681
D	1	HIS	-	expression tag	UNP P69681
D	2	HIS	-	expression tag	UNP P69681
E	-8	ALA	-	expression tag	UNP P69681
E	-7	PRO	-	expression tag	UNP P69681
E	-6	ALA	-	expression tag	UNP P69681
E	-5	VAL	-	expression tag	UNP P69681
E	-4	ALA	-	expression tag	UNP P69681
E	-3	HIS	-	expression tag	UNP P69681
E	-2	HIS	-	expression tag	UNP P69681
E	-1	HIS	-	expression tag	UNP P69681
E	0	HIS	-	expression tag	UNP P69681
E	1	HIS	-	expression tag	UNP P69681
E	2	HIS	-	expression tag	UNP P69681
F	-8	ALA	-	expression tag	UNP P69681
F	-7	PRO	-	expression tag	UNP P69681
F	-6	ALA	-	expression tag	UNP P69681
F	-5	VAL	-	expression tag	UNP P69681

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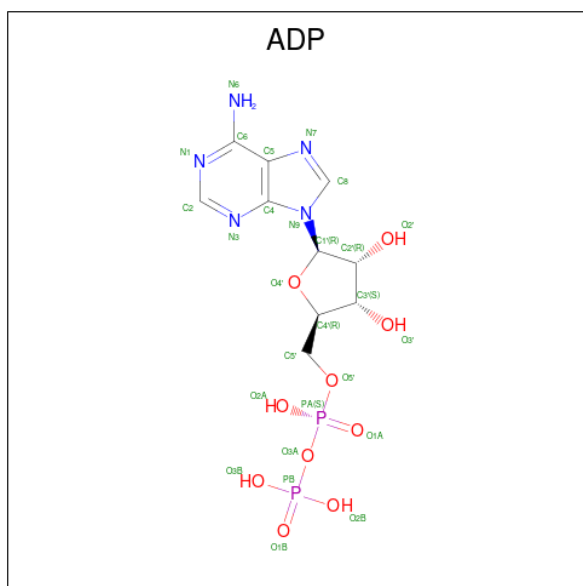
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ALA	-	expression tag	UNP P69681
F	-3	HIS	-	expression tag	UNP P69681
F	-2	HIS	-	expression tag	UNP P69681
F	-1	HIS	-	expression tag	UNP P69681
F	0	HIS	-	expression tag	UNP P69681
F	1	HIS	-	expression tag	UNP P69681
F	2	HIS	-	expression tag	UNP P69681

- Molecule 2 is a protein called Nitrogen regulatory protein P-II 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	112	Total	C	N	O	S	0	0	0
			864	552	147	164	1			
2	H	112	Total	C	N	O	S	0	0	0
			864	552	147	164	1			
2	I	112	Total	C	N	O	S	0	0	0
			864	552	147	164	1			
2	J	112	Total	C	N	O	S	0	0	0
			864	552	147	164	1			
2	K	112	Total	C	N	O	S	0	0	0
			864	552	147	164	1			
2	L	112	Total	C	N	O	S	0	0	0
			864	552	147	164	1			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

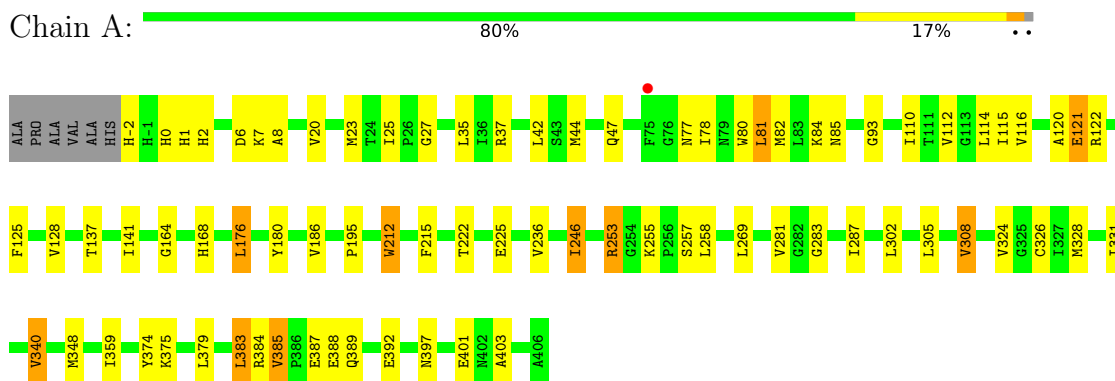
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	64	Total	O	0	0
			64	64		
4	C	82	Total	O	0	0
			82	82		
4	D	66	Total	O	0	0
			66	66		
4	E	68	Total	O	0	0
			68	68		
4	F	69	Total	O	0	0
			69	69		
4	G	19	Total	O	0	0
			19	19		
4	H	23	Total	O	0	0
			23	23		
4	I	16	Total	O	0	0
			16	16		
4	J	31	Total	O	0	0
			31	31		
4	K	21	Total	O	0	0
			21	21		
4	L	31	Total	O	0	0
			31	31		

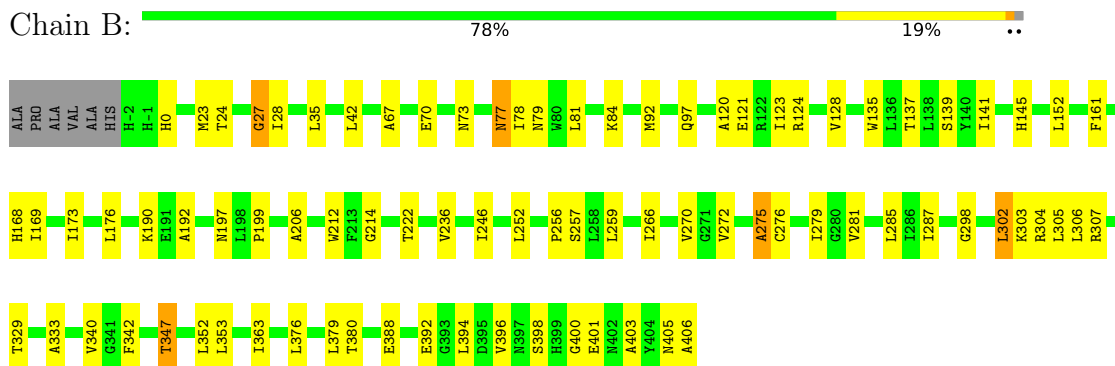
3 Residue-property plots

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.

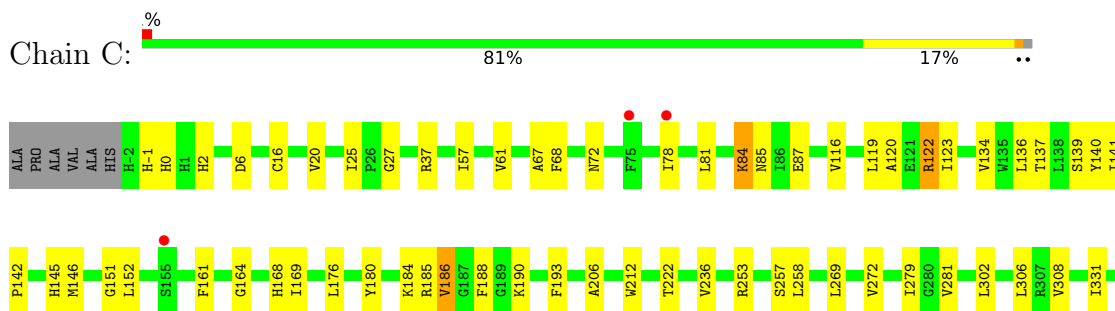
• Molecule 1: Ammonia channel



• Molecule 1: Ammonia channel

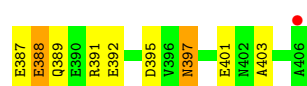
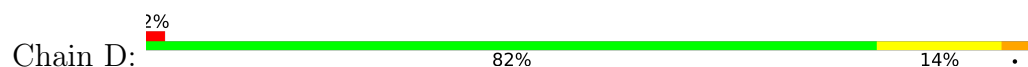


• Molecule 1: Ammonia channel

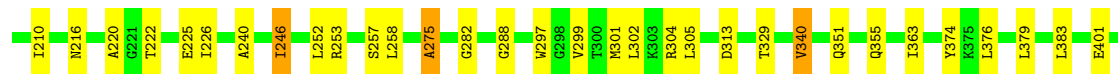
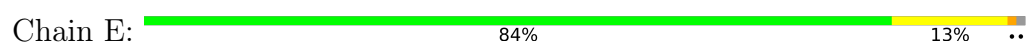




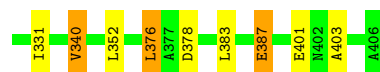
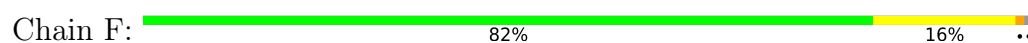
• Molecule 1: Ammonia channel



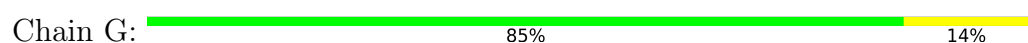
• Molecule 1: Ammonia channel

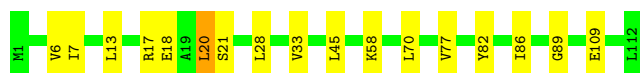


• Molecule 1: Ammonia channel

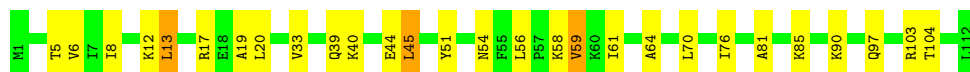
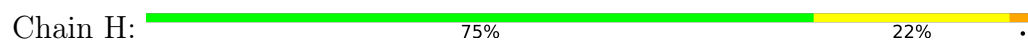


• Molecule 2: Nitrogen regulatory protein P-II 2

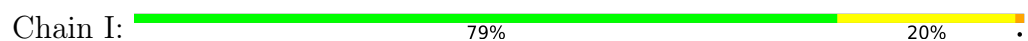




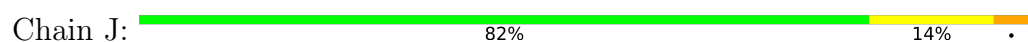
- Molecule 2: Nitrogen regulatory protein P-II 2



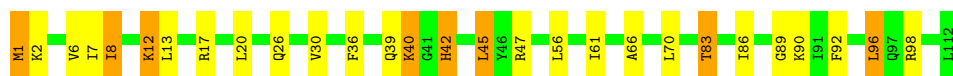
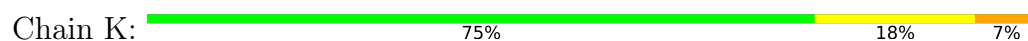
- Molecule 2: Nitrogen regulatory protein P-II 2



- Molecule 2: Nitrogen regulatory protein P-II 2



- Molecule 2: Nitrogen regulatory protein P-II 2



- Molecule 2: Nitrogen regulatory protein P-II 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.69Å 107.86Å 280.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.50) 99.8 (40.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.171 , 0.249 0.202 , 0.271	Depositor DCC
R_{free} test set	5272 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24026	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/3092	1.05	11/4209 (0.3%)
1	B	0.63	0/3092	1.06	10/4209 (0.2%)
1	C	0.59	0/3092	1.06	11/4209 (0.3%)
1	D	0.61	0/3103	1.03	8/4224 (0.2%)
1	E	0.61	0/3092	1.04	5/4209 (0.1%)
1	F	0.61	0/3092	1.04	11/4209 (0.3%)
2	G	0.52	0/873	1.00	1/1173 (0.1%)
2	H	0.51	0/873	0.99	2/1173 (0.2%)
2	I	0.51	0/873	0.98	1/1173 (0.1%)
2	J	0.57	0/873	1.02	2/1173 (0.2%)
2	K	0.55	0/873	1.03	4/1173 (0.3%)
2	L	0.59	0/873	0.97	2/1173 (0.2%)
All	All	0.60	0/23801	1.04	68/32307 (0.2%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	168	HIS	N-CA-C	9.20	121.00	110.97
1	C	168	HIS	N-CA-C	8.39	120.11	110.97
1	F	168	HIS	N-CA-C	8.29	120.24	111.03
1	A	168	HIS	N-CA-C	7.92	119.82	111.03
1	A	236	VAL	N-CA-C	7.72	117.79	110.30
1	C	403	ALA	N-CA-C	7.52	120.14	111.11
1	D	168	HIS	N-CA-C	7.39	119.03	110.97
1	A	93	GLY	N-CA-C	-7.24	105.01	111.67
1	B	403	ALA	N-CA-C	7.04	118.75	111.14
1	C	68	PHE	N-CA-C	6.88	121.96	113.50
1	D	120	ALA	N-CA-C	6.87	119.93	110.24
1	B	120	ALA	N-CA-C	6.86	119.95	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	PHE	N-CA-C	6.48	118.00	111.07
1	B	276	CYS	N-CA-C	6.37	121.82	111.37
1	A	164	GLY	N-CA-C	-6.33	104.83	112.49
1	D	236	VAL	N-CA-C	6.33	116.50	110.42
1	F	403	ALA	N-CA-C	6.32	118.69	111.11
1	F	115	ILE	N-CA-C	6.20	116.38	110.42
1	C	-1	HIS	N-CA-C	6.20	119.69	111.75
2	K	40	LYS	N-CA-C	6.11	120.91	112.90
1	F	220	ALA	N-CA-C	-6.07	105.70	113.23
1	B	79	ASN	N-CA-C	6.01	119.44	111.75
2	K	83	THR	N-CA-C	-5.97	106.61	114.31
1	C	152	LEU	N-CA-C	5.96	118.30	111.02
1	A	120	ALA	N-CA-C	5.92	118.64	110.35
2	J	83	THR	N-CA-C	-5.90	107.07	114.56
2	J	103	ARG	N-CA-C	5.86	117.67	111.28
1	B	168	HIS	N-CA-C	5.86	117.36	110.97
1	D	397	ASN	N-CA-C	5.86	117.74	111.36
2	H	40	LYS	N-CA-C	5.84	121.28	114.04
1	A	403	ALA	N-CA-C	5.82	117.30	111.07
1	A	255	LYS	N-CA-C	5.78	114.95	108.25
1	F	68	PHE	N-CA-C	5.68	121.10	113.72
1	F	161	PHE	N-CA-C	5.67	117.14	111.07
1	A	384	ARG	N-CA-C	5.62	118.12	109.07
1	D	403	ALA	N-CA-C	5.62	117.41	111.28
1	E	275	ALA	N-CA-C	5.57	120.21	113.41
1	C	120	ALA	N-CA-C	5.55	117.46	110.24
1	C	236	VAL	N-CA-C	5.54	115.68	110.30
2	H	39	GLN	N-CA-C	-5.53	100.67	109.96
2	K	8	ILE	N-CA-C	5.53	116.87	108.80
1	E	164	GLY	N-CA-C	-5.49	105.75	112.77
1	D	135	TRP	N-CA-C	5.46	117.24	111.28
1	F	275	ALA	N-CA-C	5.45	120.02	112.45
1	C	279	ILE	N-CA-C	5.45	116.98	109.46
2	G	82	TYR	N-CA-C	5.36	118.21	110.28
1	E	216	ASN	N-CA-C	5.36	116.98	111.03
1	F	-1	HIS	N-CA-C	5.35	118.59	111.75
1	C	364	VAL	N-CA-C	5.33	115.55	110.53
1	D	161	PHE	N-CA-C	5.29	116.74	110.97
2	L	89	GLY	N-CA-C	5.29	118.20	111.85
1	B	236	VAL	N-CA-C	5.28	115.49	110.53
1	B	121	GLU	N-CA-C	5.26	122.01	110.80
1	B	275	ALA	N-CA-C	5.26	119.97	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	42	HIS	N-CA-C	5.25	121.98	110.80
2	L	83	THR	N-CA-C	-5.24	107.55	114.31
2	I	8	ILE	N-CA-C	5.23	116.24	108.65
1	A	308	VAL	CB-CA-C	-5.19	103.43	110.90
1	B	214	GLY	N-CA-C	-5.18	106.22	112.49
1	B	380	THR	N-CA-C	5.18	118.06	111.69
1	F	279	ILE	N-CA-C	5.15	116.60	109.29
1	E	220	ALA	N-CA-C	-5.15	106.50	112.89
1	D	329	THR	N-CA-C	-5.14	105.76	111.36
1	A	121	GLU	N-CA-C	5.13	121.73	110.80
1	C	383	LEU	N-CA-C	5.12	117.99	111.69
1	A	383	LEU	N-CA-C	5.07	116.88	111.36
1	F	273	THR	CA-C-N	-5.01	114.58	119.64
1	F	273	THR	C-N-CA	-5.01	114.58	119.64

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	3020	0	3068	45	0
1	B	3020	0	3068	37	0
1	C	3020	0	3068	36	0
1	D	3030	0	3075	34	0
1	E	3020	0	3068	33	0
1	F	3020	0	3068	34	0
2	G	864	0	906	5	0
2	H	864	0	906	12	0
2	I	864	0	906	8	0
2	J	864	0	906	5	0
2	K	864	0	906	17	0
2	L	864	0	906	15	0
3	G	54	0	24	0	0
3	H	27	0	12	0	0
3	J	54	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	27	0	12	1	0
4	A	60	0	0	3	0
4	B	64	0	0	4	0
4	C	82	0	0	0	0
4	D	66	0	0	0	0
4	E	68	0	0	2	0
4	F	69	0	0	3	0
4	G	19	0	0	0	0
4	H	23	0	0	0	0
4	I	16	0	0	0	0
4	J	31	0	0	0	0
4	K	21	0	0	1	0
4	L	31	0	0	0	0
All	All	24026	0	23923	243	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 5.

All (243) 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:E:253:ARG:HE	2:K:45:LEU:HD11	1.45	0.80
1:C:72:ASN:O	1:C:145:HIS:HE1	1.70	0.75
1:C:186:VAL:HG11	1:C:387:GLU:HG3	1.72	0.71
1:D:392:GLU:HG3	1:D:397:ASN:HD21	1.55	0.71
1:A:186:VAL:HG21	1:A:387:GLU:HG3	1.73	0.70
1:A:225:GLU:OE2	1:E:2:HIS:HE1	1.76	0.68
2:L:12:LYS:HE3	2:L:83:THR:HG22	1.77	0.67
1:B:307:ARG:HA	4:B:462:HOH:O	1.95	0.66
1:B:394:LEU:O	1:B:398:SER:HB2	1.95	0.65
1:A:84:LYS:O	1:A:85:ASN:HB2	1.95	0.64
1:A:0:HIS:CD2	1:E:340:VAL:HG21	2.34	0.63
1:E:282:GLY:HA2	1:F:82:MET:HE1	1.81	0.62
1:F:11:ALA:O	1:F:15:ILE:HG12	2.00	0.62
1:B:304:ARG:HA	4:B:462:HOH:O	2.00	0.61
1:A:258:LEU:HD22	1:B:42:LEU:HD22	1.83	0.61
1:D:137:THR:HA	1:D:141:ILE:HD12	1.81	0.61
1:F:77:ASN:C	1:F:77:ASN:HD22	2.09	0.61
1:A:385:VAL:HG13	1:A:389:GLN:HB2	1.83	0.60
2:I:3:LEU:HB2	2:I:96:LEU:HD12	1.84	0.60
1:A:331:ILE:HA	1:A:348:MET:HE2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LYS:O	1:C:85:ASN:HB2	2.00	0.59
1:A:2:HIS:HE1	1:E:225:GLU:OE2	1.85	0.59
1:C:0:HIS:CD2	1:F:340:VAL:HG21	2.38	0.59
1:B:347:THR:HG21	4:B:459:HOH:O	2.02	0.59
2:K:1:MET:HE2	2:K:66:ALA:HA	1.84	0.58
1:E:0:HIS:CD2	1:E:0:HIS:H	2.20	0.58
1:F:331:ILE:HG13	1:F:352:LEU:HD21	1.86	0.58
2:K:7:ILE:O	2:K:89:GLY:HA3	2.03	0.58
2:L:6:VAL:HG12	2:L:8:ILE:HG23	1.86	0.57
1:F:378:ASP:HB2	1:F:383:LEU:HG	1.87	0.57
1:C:180:TYR:CE2	1:C:308:VAL:HG22	2.40	0.57
2:K:17:ARG:HH22	2:L:53:VAL:HG11	1.69	0.57
1:B:396:VAL:O	1:B:400:GLY:HA2	2.05	0.57
1:C:0:HIS:HD2	1:F:340:VAL:HG21	1.70	0.56
1:D:257:SER:HB2	1:E:401:GLU:CD	2.31	0.56
1:C:16:CYS:O	1:C:20:VAL:HG23	2.07	0.55
1:E:178:GLY:O	1:E:182:ILE:HG12	2.06	0.55
2:K:96:LEU:HD21	2:L:92:PHE:HB3	1.87	0.55
1:A:125:PHE:O	1:A:128:VAL:HG12	2.07	0.55
2:K:39:GLN:HB2	2:K:86:ILE:HG22	1.88	0.54
1:D:42:LEU:HD22	1:F:258:LEU:HD22	1.89	0.54
1:B:35:LEU:HD21	1:B:259:LEU:HD11	1.89	0.54
1:D:72:ASN:O	1:D:145:HIS:HE1	1.91	0.54
1:E:258:LEU:CD1	1:F:45:LEU:HB2	2.37	0.54
1:E:84:LYS:O	1:E:85:ASN:HB2	2.08	0.53
1:C:388:GLU:CD	1:C:388:GLU:H	2.16	0.53
1:A:137:THR:HA	1:A:141:ILE:HD12	1.90	0.53
1:A:112:VAL:HA	1:A:115:ILE:HD12	1.90	0.53
1:C:164:GLY:O	1:C:169:ILE:HG13	2.09	0.53
1:A:110:ILE:O	1:A:114:LEU:HG	2.09	0.53
1:B:173:ILE:HD11	1:B:363:ILE:HG12	1.91	0.53
1:A:78:ILE:HG23	1:A:81:LEU:HD23	1.90	0.53
1:B:169:ILE:O	1:B:173:ILE:HG12	2.09	0.53
1:C:119:LEU:HD13	1:C:123:ILE:HD13	1.90	0.53
1:A:20:VAL:O	1:A:23:MET:HB2	2.09	0.52
2:H:19:ALA:HB1	2:H:76:ILE:HG12	1.91	0.52
4:B:463:HOH:O	1:D:-1:HIS:HB3	2.09	0.52
1:B:257:SER:HB2	1:C:401:GLU:CD	2.35	0.52
1:F:319:GLY:O	1:F:323:ILE:HG13	2.10	0.52
2:G:7:ILE:O	2:G:89:GLY:HA3	2.10	0.52
2:K:30:VAL:HG22	2:K:61:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:HIS:HB3	4:A:434:HOH:O	2.09	0.51
1:F:236:VAL:HG21	1:F:281:VAL:HG23	1.91	0.51
1:B:67:ALA:O	1:B:145:HIS:HD2	1.94	0.51
1:B:73:ASN:HB3	1:B:152:LEU:HB2	1.92	0.51
1:C:122:ARG:HD2	1:C:185:ARG:HG2	1.91	0.51
1:C:137:THR:HA	1:C:141:ILE:HD12	1.92	0.51
1:A:374:TYR:HB3	1:A:383:LEU:HD11	1.93	0.51
1:A:257:SER:HB2	1:B:401:GLU:CD	2.36	0.50
1:D:331:ILE:HG13	1:D:352:LEU:HD21	1.93	0.50
1:A:326:CYS:HB2	1:A:359:ILE:HD11	1.94	0.50
1:A:44:MET:SD	1:A:116:VAL:HG12	2.51	0.50
1:C:134:VAL:HG21	1:C:376:LEU:HD13	1.93	0.50
1:C:2:HIS:HE1	1:F:225:GLU:OE2	1.93	0.49
1:A:-2:HIS:CE1	1:A:1:HIS:HB2	2.48	0.49
1:E:87:GLU:HG3	4:E:435:HOH:O	2.12	0.49
1:B:388:GLU:O	1:B:392:GLU:HG2	2.12	0.49
2:L:1:MET:HE1	2:L:109:GLU:HG3	1.95	0.49
1:C:67:ALA:O	1:C:145:HIS:HD2	1.96	0.49
1:B:78:ILE:O	1:B:81:LEU:HD13	2.13	0.48
1:E:374:TYR:HB3	1:E:383:LEU:HD11	1.94	0.48
2:L:1:MET:HE2	2:L:66:ALA:HA	1.95	0.48
2:J:96:LEU:HD21	2:K:92:PHE:HB3	1.95	0.48
1:B:0:HIS:CD2	1:D:226:ILE:HD12	2.49	0.48
1:E:240:ALA:HB3	1:E:288:GLY:HA3	1.95	0.48
2:K:1:MET:CE	2:K:66:ALA:HA	2.44	0.48
1:A:77:ASN:HB2	4:A:427:HOH:O	2.12	0.48
1:A:176:LEU:HD22	1:A:180:TYR:CE1	2.48	0.48
1:A:324:VAL:O	1:A:328:MET:HG3	2.13	0.48
1:E:253:ARG:NE	2:K:45:LEU:HD11	2.21	0.48
2:J:109:GLU:CD	2:J:109:GLU:H	2.21	0.48
1:D:42:LEU:HD22	1:F:258:LEU:CD2	2.43	0.48
1:B:137:THR:HA	1:B:141:ILE:HD12	1.94	0.48
1:F:147:VAL:HG22	1:F:153:LEU:HD12	1.95	0.47
2:H:44:GLU:HG3	2:H:54:ASN:ND2	2.29	0.47
1:F:246:ILE:O	1:F:250:TRP:HB2	2.14	0.47
1:B:192:ALA:HA	2:H:51:TYR:CE1	2.49	0.47
2:G:20:LEU:HD23	2:G:28:LEU:HD23	1.97	0.47
1:F:-2:HIS:N	4:F:469:HOH:O	2.47	0.47
1:E:173:ILE:HG13	1:E:363:ILE:HA	1.97	0.46
1:D:11:ALA:O	1:D:15:ILE:HG12	2.15	0.46
1:E:103:PHE:CZ	1:E:107:PHE:HE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HG13	1:B:124:ARG:N	2.30	0.46
1:A:42:LEU:HD22	1:C:258:LEU:CD2	2.45	0.46
1:A:42:LEU:HD22	1:C:258:LEU:HD23	1.97	0.46
1:F:387:GLU:HG2	4:F:425:HOH:O	2.13	0.46
1:C:375:LYS:HA	1:C:375:LYS:HD3	1.71	0.46
2:J:38:ARG:HB3	2:J:86:ILE:HD11	1.98	0.46
2:K:6:VAL:HG12	2:K:8:ILE:HG23	1.96	0.46
2:L:106:GLU:O	2:L:111:ALA:HB2	2.16	0.46
1:F:35:LEU:HD21	1:F:259:LEU:HD11	1.97	0.46
1:C:184:LYS:HD3	1:C:188:PHE:CD2	2.50	0.46
1:F:110:ILE:O	1:F:114:LEU:HG	2.16	0.46
2:I:6:VAL:HG21	2:I:77:VAL:HG11	1.98	0.46
1:A:35:LEU:HA	1:A:195:PRO:HB3	1.98	0.45
1:D:84:LYS:HE2	1:D:85:ASN:HD21	1.81	0.45
1:D:297:TRP:CD1	1:D:301:MET:HG3	2.51	0.45
1:D:39:LYS:NZ	1:D:391:ARG:O	2.48	0.45
1:D:75:PHE:CZ	1:D:142:PRO:HG3	2.52	0.45
1:F:47:GLN:HB3	1:F:116:VAL:HG11	1.97	0.45
2:K:98:ARG:HG3	4:K:122:HOH:O	2.16	0.45
2:K:36:PHE:CZ	2:K:40:LYS:HG2	2.52	0.45
1:E:123:ILE:HG12	1:E:128:VAL:HG23	1.99	0.45
1:C:306:LEU:HB3	1:C:308:VAL:HG23	1.98	0.45
1:D:123:ILE:HD12	1:D:128:VAL:HG23	1.97	0.45
2:L:14:GLU:OE1	2:L:14:GLU:HA	2.17	0.45
1:D:20:VAL:O	1:D:23:MET:HB2	2.17	0.45
2:H:6:VAL:HG12	2:H:8:ILE:HG23	1.99	0.45
2:I:66:ALA:HB3	2:I:69:GLN:HG3	1.99	0.45
1:A:82:MET:HE3	1:C:281:VAL:HG13	1.97	0.45
1:B:81:LEU:O	1:B:84:LYS:HG2	2.17	0.45
1:B:275:ALA:HB2	1:B:329:THR:OG1	2.16	0.45
1:F:13:MET:HG3	1:F:95:ILE:HG21	1.99	0.45
2:H:13:LEU:HG	2:H:59:VAL:HG11	1.98	0.45
1:B:77:ASN:C	1:B:77:ASN:HD22	2.25	0.45
2:H:33:VAL:HG23	2:H:58:LYS:HB2	1.99	0.45
1:A:84:LYS:HE2	4:A:432:HOH:O	2.16	0.44
1:B:298:GLY:HA2	1:B:302:LEU:HB3	2.00	0.44
1:A:401:GLU:CD	1:C:257:SER:HB2	2.42	0.44
1:B:92:MET:HB2	1:B:97:GLN:HG3	1.97	0.44
1:C:331:ILE:HG13	1:C:352:LEU:HD21	1.99	0.44
1:E:299:VAL:HG12	1:E:313:ASP:HB3	2.00	0.44
1:B:340:VAL:HG21	1:D:0:HIS:ND1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:TRP:CG	1:C:269:LEU:HD22	2.52	0.44
2:L:13:LEU:HG	2:L:59:VAL:HG11	2.00	0.44
1:E:351:GLN:O	1:E:355:GLN:HG2	2.18	0.44
2:K:12:LYS:NZ	2:K:83:THR:HG22	2.31	0.44
1:B:24:THR:HA	1:B:28:ILE:HG22	1.98	0.44
1:B:246:ILE:HG23	1:B:256:PRO:HB3	1.98	0.44
2:J:12:LYS:HD2	2:J:83:THR:CG2	2.47	0.44
1:A:375:LYS:O	1:A:379:LEU:HG	2.18	0.44
1:F:80:TRP:CD1	1:F:86:ILE:HG13	2.53	0.44
1:F:134:VAL:HG21	1:F:376:LEU:HD12	1.99	0.44
1:C:57:ILE:O	1:C:61:VAL:HG23	2.17	0.44
2:H:12:LYS:HD2	2:H:81:ALA:O	2.17	0.44
2:I:39:GLN:HB2	2:I:86:ILE:HG22	2.00	0.44
1:B:135:TRP:O	1:B:139:SER:HB3	2.17	0.44
2:H:103:ARG:HG2	2:H:104:THR:HG23	1.98	0.44
1:D:25:ILE:HA	1:D:26:PRO:HA	1.88	0.43
1:D:40:ASN:HA	1:D:395:ASP:OD1	2.17	0.43
1:D:84:LYS:HE2	1:D:85:ASN:ND2	2.33	0.43
1:B:279:ILE:HD13	1:B:287:ILE:HD12	2.00	0.43
1:C:186:VAL:HG22	1:C:390:GLU:CD	2.43	0.43
1:E:11:ALA:O	1:E:15:ILE:HG12	2.19	0.43
1:E:137:THR:HA	1:E:141:ILE:HD12	1.99	0.43
1:E:210:ILE:HG13	1:F:22:PHE:CD1	2.54	0.43
2:L:7:ILE:HD12	2:L:92:PHE:HE2	1.84	0.43
1:D:388:GLU:O	1:D:392:GLU:HG2	2.18	0.43
1:E:297:TRP:CD1	1:E:301:MET:HG3	2.54	0.43
1:D:81:LEU:O	1:D:84:LYS:HG2	2.19	0.43
1:E:16:CYS:O	1:E:20:VAL:HG23	2.19	0.43
1:E:84:LYS:HA	4:E:427:HOH:O	2.19	0.43
1:E:257:SER:HB2	1:F:401:GLU:CD	2.43	0.43
1:E:313:ASP:HB2	2:K:47:ARG:NH1	2.33	0.43
1:C:146:MET:HA	1:C:151:GLY:HA3	2.01	0.42
2:I:70:LEU:HD11	2:I:93:VAL:HG11	2.01	0.42
2:K:17:ARG:NH2	2:L:53:VAL:HG11	2.31	0.42
1:C:142:PRO:O	1:C:146:MET:HG3	2.20	0.42
1:D:205:THR:HG23	1:D:266:ILE:HD11	2.01	0.42
1:D:224:ASN:ND2	1:D:227:ALA:H	2.17	0.42
2:G:6:VAL:HG21	2:G:77:VAL:HG11	2.00	0.42
2:H:5:THR:HA	2:H:61:ILE:O	2.19	0.42
1:C:139:SER:HB2	1:C:369:VAL:HG11	2.00	0.42
2:K:26:GLN:HE21	2:K:26:GLN:HB3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASP:OD2	1:A:8:ALA:HB3	2.19	0.42
1:A:212:TRP:CE3	1:A:269:LEU:HD13	2.55	0.42
1:B:333:ALA:HB3	1:B:342:PHE:CE1	2.55	0.42
1:B:197:ASN:OD1	1:B:199:PRO:HD2	2.20	0.42
1:C:141:ILE:HB	1:C:142:PRO:HD3	2.02	0.42
1:F:47:GLN:O	1:F:51:THR:HG23	2.20	0.42
2:J:50:GLU:O	2:J:50:GLU:HG3	2.20	0.42
1:F:246:ILE:HD13	1:F:246:ILE:HA	1.92	0.42
2:L:9:LYS:HE3	2:L:87:GLY:C	2.45	0.42
1:A:283:GLY:O	1:A:287:ILE:HG13	2.19	0.42
1:B:266:ILE:O	1:B:270:VAL:HG23	2.20	0.41
1:D:246:ILE:HD13	1:D:246:ILE:HA	1.89	0.41
1:F:1:HIS:HD2	4:F:444:HOH:O	2.03	0.41
2:H:64:ALA:HB2	2:I:92:PHE:HE1	1.85	0.41
1:A:47:GLN:HG2	1:A:128:VAL:HG11	2.02	0.41
1:A:80:TRP:HD1	1:A:85:ASN:HB2	1.85	0.41
1:D:401:GLU:HG2	2:L:46:TYR:CE1	2.54	0.41
1:E:126:SER:O	1:E:130:ILE:HG13	2.21	0.41
2:G:17:ARG:HH12	2:G:18:GLU:HG3	1.85	0.41
1:B:161:PHE:CD1	1:D:-3:HIS:N	2.84	0.41
1:C:37:ARG:NH2	1:C:193:PHE:HE2	2.18	0.41
1:D:67:ALA:O	1:D:145:HIS:HD2	2.03	0.41
1:F:16:CYS:O	1:F:20:VAL:HG23	2.20	0.41
1:F:137:THR:HA	1:F:141:ILE:HD12	2.01	0.41
2:H:45:LEU:C	2:H:45:LEU:HD23	2.45	0.41
1:A:212:TRP:O	1:A:215:PHE:HB3	2.20	0.41
1:B:23:MET:O	1:B:27:GLY:HA3	2.21	0.41
1:F:304:ARG:HD2	1:F:304:ARG:HA	1.84	0.41
1:F:59:TRP:HA	1:F:63:GLY:HA3	2.03	0.41
1:D:165:THR:OG1	1:D:166:VAL:N	2.53	0.41
1:D:180:TYR:CZ	1:D:308:VAL:HG22	2.55	0.41
1:D:275:ALA:HB2	1:D:329:THR:OG1	2.19	0.41
1:A:78:ILE:O	1:A:78:ILE:CG2	2.68	0.41
1:C:136:LEU:HD12	1:C:140:TYR:HB3	2.03	0.41
2:H:97:GLN:HE21	2:I:95:GLU:HB2	1.86	0.41
1:A:246:ILE:HD13	1:A:246:ILE:HA	1.89	0.41
1:D:188:PHE:HA	1:D:193:PHE:CE1	2.56	0.41
1:E:134:VAL:HG21	1:E:376:LEU:HD23	2.03	0.41
1:E:275:ALA:HB2	1:E:329:THR:OG1	2.20	0.41
1:F:317:VAL:O	1:F:321:CYS:HB2	2.21	0.41
2:L:1:MET:CE	2:L:66:ALA:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HE	1:A:253:ARG:HA	1.86	0.41
1:A:340:VAL:HG21	1:E:0:HIS:ND1	2.36	0.41
1:B:206:ALA:CB	1:C:25:ILE:HG22	2.51	0.41
2:G:33:VAL:HG23	2:G:58:LYS:HB2	2.02	0.41
1:A:37:ARG:HH21	1:A:121:GLU:CD	2.29	0.40
1:A:78:ILE:HD13	1:A:78:ILE:HA	1.93	0.40
1:D:224:ASN:HD22	1:D:224:ASN:C	2.29	0.40
2:I:5:THR:HB	2:I:92:PHE:HB2	2.02	0.40
1:F:309:ASP:O	1:F:311:PRO:HD3	2.20	0.40
1:B:67:ALA:O	1:B:145:HIS:CD2	2.74	0.40
1:B:405:ASN:O	1:B:406:ALA:C	2.65	0.40
1:D:385:VAL:HG13	1:D:389:GLN:HB2	2.04	0.40
1:E:80:TRP:HA	1:E:84:LYS:O	2.21	0.40
1:E:246:ILE:HD13	1:E:246:ILE:HA	1.89	0.40
1:A:7:LYS:HE3	1:C:6:ASP:OD2	2.22	0.40
1:A:25:ILE:HG22	1:C:206:ALA:CB	2.52	0.40
1:A:392:GLU:HB3	1:A:397:ASN:HD21	1.87	0.40
2:L:90:LYS:HE2	3:L:1600:ADP:O3B	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	407/415 (98%)	384 (94%)	22 (5%)	1 (0%)	43	63
1	B	407/415 (98%)	388 (95%)	18 (4%)	1 (0%)	43	63
1	C	407/415 (98%)	380 (93%)	26 (6%)	1 (0%)	43	63
1	D	408/415 (98%)	385 (94%)	22 (5%)	1 (0%)	43	63
1	E	407/415 (98%)	379 (93%)	27 (7%)	1 (0%)	43	63
1	F	407/415 (98%)	382 (94%)	22 (5%)	3 (1%)	18	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
2	H	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
2	I	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	14	27
2	J	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
2	K	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	27
2	L	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
All	All	3103/3162 (98%)	2927 (94%)	166 (5%)	10 (0%)	36	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	108	ASP
1	B	27	GLY
1	C	27	GLY
1	D	27	GLY
1	E	27	GLY
2	K	42	HIS
1	A	27	GLY
1	F	188	PHE
1	F	72	ASN
1	F	27	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	301/304 (99%)	287 (95%)	14 (5%)	23	47
1	B	301/304 (99%)	281 (93%)	20 (7%)	15	32
1	C	301/304 (99%)	285 (95%)	16 (5%)	20	42
1	D	302/304 (99%)	281 (93%)	21 (7%)	14	29
1	E	301/304 (99%)	288 (96%)	13 (4%)	26	51
1	F	301/304 (99%)	288 (96%)	13 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	91/91 (100%)	84 (92%)	7 (8%)	12	25
2	H	91/91 (100%)	82 (90%)	9 (10%)	7	16
2	I	91/91 (100%)	82 (90%)	9 (10%)	7	16
2	J	91/91 (100%)	76 (84%)	15 (16%)	2	4
2	K	91/91 (100%)	81 (89%)	10 (11%)	6	13
2	L	91/91 (100%)	80 (88%)	11 (12%)	5	10
All	All	2353/2370 (99%)	2195 (93%)	158 (7%)	15	31

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	122	ARG
1	A	176	LEU
1	A	212	TRP
1	A	222	THR
1	A	246	ILE
1	A	253	ARG
1	A	281	VAL
1	A	302	LEU
1	A	305	LEU
1	A	308	VAL
1	A	340	VAL
1	A	385	VAL
1	A	388	GLU
1	B	70	GLU
1	B	77	ASN
1	B	128	VAL
1	B	176	LEU
1	B	190	LYS
1	B	212	TRP
1	B	222	THR
1	B	252	LEU
1	B	272	VAL
1	B	281	VAL
1	B	285	LEU
1	B	302	LEU
1	B	303	LYS
1	B	305	LEU
1	B	306	LEU

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Mol	Chain	Res	Type
1	B	347	THR
1	B	352	LEU
1	B	353	LEU
1	B	376	LEU
1	B	379	LEU
1	C	78	ILE
1	C	81	LEU
1	C	84	LYS
1	C	87	GLU
1	C	116	VAL
1	C	122	ARG
1	C	176	LEU
1	C	186	VAL
1	C	190	LYS
1	C	222	THR
1	C	253	ARG
1	C	272	VAL
1	C	302	LEU
1	C	356	LEU
1	C	364	VAL
1	C	388	GLU
1	D	-1	HIS
1	D	4	VAL
1	D	78	ILE
1	D	81	LEU
1	D	122	ARG
1	D	123	ILE
1	D	124	ARG
1	D	156	HIS
1	D	176	LEU
1	D	212	TRP
1	D	222	THR
1	D	224	ASN
1	D	226	ILE
1	D	246	ILE
1	D	285	LEU
1	D	301	MET
1	D	308	VAL
1	D	340	VAL
1	D	385	VAL
1	D	387	GLU
1	D	388	GLU

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Mol	Chain	Res	Type
1	E	0	HIS
1	E	84	LYS
1	E	122	ARG
1	E	176	LEU
1	E	222	THR
1	E	226	ILE
1	E	246	ILE
1	E	252	LEU
1	E	302	LEU
1	E	304	ARG
1	E	305	LEU
1	E	340	VAL
1	E	379	LEU
1	F	77	ASN
1	F	81	LEU
1	F	116	VAL
1	F	122	ARG
1	F	128	VAL
1	F	176	LEU
1	F	212	TRP
1	F	222	THR
1	F	302	LEU
1	F	307	ARG
1	F	340	VAL
1	F	376	LEU
1	F	387	GLU
2	G	13	LEU
2	G	20	LEU
2	G	21	SER
2	G	45	LEU
2	G	70	LEU
2	G	86	ILE
2	G	109	GLU
2	H	13	LEU
2	H	17	ARG
2	H	20	LEU
2	H	45	LEU
2	H	56	LEU
2	H	59	VAL
2	H	70	LEU
2	H	85	LYS
2	H	90	LYS

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Mol	Chain	Res	Type
2	I	1	MET
2	I	13	LEU
2	I	14	GLU
2	I	15	ASP
2	I	20	LEU
2	I	34	LYS
2	I	53	VAL
2	I	76	ILE
2	I	96	LEU
2	J	6	VAL
2	J	13	LEU
2	J	17	ARG
2	J	26	GLN
2	J	40	LYS
2	J	45	LEU
2	J	50	GLU
2	J	69	GLN
2	J	70	LEU
2	J	74	ILE
2	J	76	ILE
2	J	96	LEU
2	J	100	ILE
2	J	109	GLU
2	J	112	LEU
2	K	1	MET
2	K	2	LYS
2	K	12	LYS
2	K	13	LEU
2	K	20	LEU
2	K	45	LEU
2	K	56	LEU
2	K	70	LEU
2	K	90	LYS
2	K	96	LEU
2	L	7	ILE
2	L	13	LEU
2	L	17	ARG
2	L	20	LEU
2	L	26	GLN
2	L	45	LEU
2	L	56	LEU
2	L	70	LEU

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Mol	Chain	Res	Type
2	L	76	ILE
2	L	79	LYS
2	L	99	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	79	ASN
1	A	85	ASN
1	A	97	GLN
1	A	104	GLN
1	A	145	HIS
1	A	216	ASN
1	A	389	GLN
1	A	397	ASN
1	A	402	ASN
1	B	77	ASN
1	B	79	ASN
1	B	145	HIS
1	B	156	HIS
1	C	-2	HIS
1	C	2	HIS
1	C	73	ASN
1	C	79	ASN
1	C	104	GLN
1	C	145	HIS
1	C	156	HIS
1	C	402	ASN
1	D	0	HIS
1	D	85	ASN
1	D	145	HIS
1	D	156	HIS
1	D	224	ASN
1	D	351	GLN
1	D	397	ASN
1	E	0	HIS
1	E	2	HIS
1	E	79	ASN
1	E	104	GLN
1	E	145	HIS
1	E	351	GLN

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Mol	Chain	Res	Type
1	E	389	GLN
1	E	397	ASN
1	F	1	HIS
1	F	77	ASN
1	F	79	ASN
1	F	104	GLN
1	F	145	HIS
1	F	216	ASN
1	F	402	ASN
2	G	26	GLN
2	G	54	ASN
2	J	42	HIS
2	K	26	GLN
2	K	97	GLN

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	G	1400	-	28,29,29	1.53	5 (17%)	43,45,45	1.73	9 (20%)
3	ADP	H	1300	-	28,29,29	1.51	5 (17%)	43,45,45	1.77	7 (16%)
3	ADP	G	1200	-	28,29,29	1.43	5 (17%)	43,45,45	1.85	12 (27%)
3	ADP	J	1500	-	28,29,29	1.47	5 (17%)	43,45,45	1.90	11 (25%)
3	ADP	L	1600	-	28,29,29	1.52	6 (21%)	43,45,45	1.71	9 (20%)
3	ADP	J	1700	-	28,29,29	1.52	6 (21%)	43,45,45	1.79	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	G	1400	-	-	0/16/32/32	0/3/3/3
3	ADP	H	1300	-	-	0/16/32/32	0/3/3/3
3	ADP	G	1200	-	-	0/16/32/32	0/3/3/3
3	ADP	J	1500	-	-	1/16/32/32	0/3/3/3
3	ADP	L	1600	-	-	0/16/32/32	0/3/3/3
3	ADP	J	1700	-	-	0/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1700	ADP	C5-C4	5.14	1.48	1.39
3	G	1400	ADP	C5-C4	5.11	1.48	1.39
3	H	1300	ADP	C5-C4	5.02	1.48	1.39
3	L	1600	ADP	C5-C4	4.81	1.47	1.39
3	J	1500	ADP	C5-C4	4.77	1.47	1.39
3	G	1200	ADP	C5-C4	4.45	1.47	1.39
3	J	1700	ADP	C5-C6	2.98	1.49	1.41
3	G	1400	ADP	C5-C6	2.98	1.49	1.41
3	J	1500	ADP	C5-C6	2.83	1.48	1.41
3	H	1300	ADP	C5-C6	2.83	1.48	1.41
3	L	1600	ADP	C5-C6	2.77	1.48	1.41
3	L	1600	ADP	PA-O3A	2.77	1.62	1.59
3	G	1200	ADP	C5-C6	2.65	1.48	1.41
3	L	1600	ADP	C8-N7	2.50	1.36	1.31
3	J	1500	ADP	PA-O3A	2.49	1.62	1.59
3	G	1200	ADP	PA-O3A	2.44	1.62	1.59
3	G	1400	ADP	C8-N7	2.43	1.36	1.31
3	J	1500	ADP	C8-N7	2.42	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1400	ADP	PA-O3A	2.38	1.62	1.59
3	H	1300	ADP	C8-N7	2.36	1.36	1.31
3	L	1600	ADP	C5-N7	-2.34	1.34	1.39
3	H	1300	ADP	C5-N7	-2.34	1.34	1.39
3	H	1300	ADP	PA-O3A	2.26	1.61	1.59
3	J	1700	ADP	C8-N7	2.25	1.36	1.31
3	G	1400	ADP	C5-N7	-2.25	1.35	1.39
3	G	1200	ADP	C5-N7	-2.24	1.35	1.39
3	L	1600	ADP	C4-N9	-2.22	1.33	1.37
3	J	1700	ADP	PA-O3A	2.16	1.61	1.59
3	J	1700	ADP	C5-N7	-2.16	1.35	1.39
3	J	1700	ADP	C4-N9	-2.11	1.33	1.37
3	J	1500	ADP	C5-N7	-2.07	1.35	1.39
3	G	1200	ADP	C8-N7	2.07	1.35	1.31

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1300	ADP	C5-C4-N3	-6.01	118.44	126.72
3	J	1500	ADP	C5-C4-N3	-5.74	118.81	126.72
3	G	1200	ADP	C5-C4-N3	-5.64	118.95	126.72
3	J	1700	ADP	C5-C4-N3	-5.54	119.09	126.72
3	L	1600	ADP	C5-C4-N3	-5.52	119.12	126.72
3	G	1400	ADP	C5-C4-N3	-5.33	119.38	126.72
3	G	1200	ADP	N3-C4-N9	4.64	135.05	127.17
3	H	1300	ADP	N3-C4-N9	4.63	135.05	127.17
3	J	1700	ADP	N3-C4-N9	4.35	134.56	127.17
3	G	1400	ADP	N3-C4-N9	4.30	134.48	127.17
3	J	1500	ADP	N3-C4-N9	4.22	134.35	127.17
3	J	1500	ADP	C4-C5-N7	-4.08	105.92	110.58
3	L	1600	ADP	N3-C4-N9	4.07	134.09	127.17
3	J	1500	ADP	C2-N3-C4	3.96	121.50	111.83
3	J	1500	ADP	N3-C2-N1	-3.87	122.72	128.58
3	G	1200	ADP	C2-N3-C4	3.80	121.10	111.83
3	L	1600	ADP	C2-N3-C4	3.76	121.01	111.83
3	G	1200	ADP	N3-C2-N1	-3.71	122.97	128.58
3	H	1300	ADP	C2-N3-C4	3.69	120.84	111.83
3	L	1600	ADP	N3-C2-N1	-3.64	123.07	128.58
3	J	1700	ADP	C2-N3-C4	3.60	120.62	111.83
3	G	1400	ADP	C2-N3-C4	3.57	120.56	111.83
3	H	1300	ADP	C4-C5-N7	-3.57	106.50	110.58
3	J	1700	ADP	C4-C5-N7	-3.44	106.64	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1400	ADP	C4-C5-N7	-3.44	106.65	110.58
3	G	1400	ADP	N3-C2-N1	-3.43	123.39	128.58
3	J	1700	ADP	N3-C2-N1	-3.39	123.45	128.58
3	G	1200	ADP	C4-C5-N7	-3.32	106.78	110.58
3	H	1300	ADP	N3-C2-N1	-3.30	123.58	128.58
3	L	1600	ADP	C4-C5-N7	-3.30	106.81	110.58
3	J	1500	ADP	C5-N7-C8	2.94	108.08	103.45
3	G	1200	ADP	C4-N9-C8	2.94	108.82	105.74
3	J	1500	ADP	C6-C5-N7	2.69	137.27	132.09
3	G	1400	ADP	C4-N9-C8	2.68	108.55	105.74
3	G	1200	ADP	C5-N7-C8	2.61	107.56	103.45
3	G	1400	ADP	C5-N7-C8	2.55	107.45	103.45
3	J	1700	ADP	C4-N9-C8	2.52	108.39	105.74
3	H	1300	ADP	C5-N7-C8	2.51	107.40	103.45
3	J	1700	ADP	O3A-PA-O1A	-2.43	103.40	110.70
3	J	1700	ADP	C5-N7-C8	2.40	107.22	103.45
3	J	1500	ADP	C4-N9-C8	2.39	108.25	105.74
3	L	1600	ADP	C6-C5-N7	2.35	136.63	132.09
3	J	1500	ADP	C2-N1-C6	2.26	122.45	118.73
3	G	1400	ADP	C6-C5-N7	2.23	136.39	132.09
3	G	1400	ADP	C2-N1-C6	2.20	122.35	118.73
3	G	1200	ADP	N9-C8-N7	-2.19	110.83	113.94
3	J	1700	ADP	C2-N1-C6	2.18	122.31	118.73
3	G	1200	ADP	C2-N1-C6	2.17	122.30	118.73
3	G	1200	ADP	O3A-PA-O1A	-2.17	104.19	110.70
3	H	1300	ADP	C4-N9-C8	2.16	108.01	105.74
3	J	1500	ADP	N9-C8-N7	-2.13	110.91	113.94
3	G	1200	ADP	C6-C5-N7	2.13	136.20	132.09
3	J	1500	ADP	O3A-PA-O1A	-2.13	104.30	110.70
3	L	1600	ADP	C2-N1-C6	2.13	122.22	118.73
3	L	1600	ADP	C5-N7-C8	2.12	106.78	103.45
3	J	1700	ADP	C6-C5-N7	2.10	136.13	132.09
3	L	1600	ADP	C4-N9-C8	2.07	107.91	105.74
3	G	1200	ADP	O3B-PB-O2B	2.06	115.51	107.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

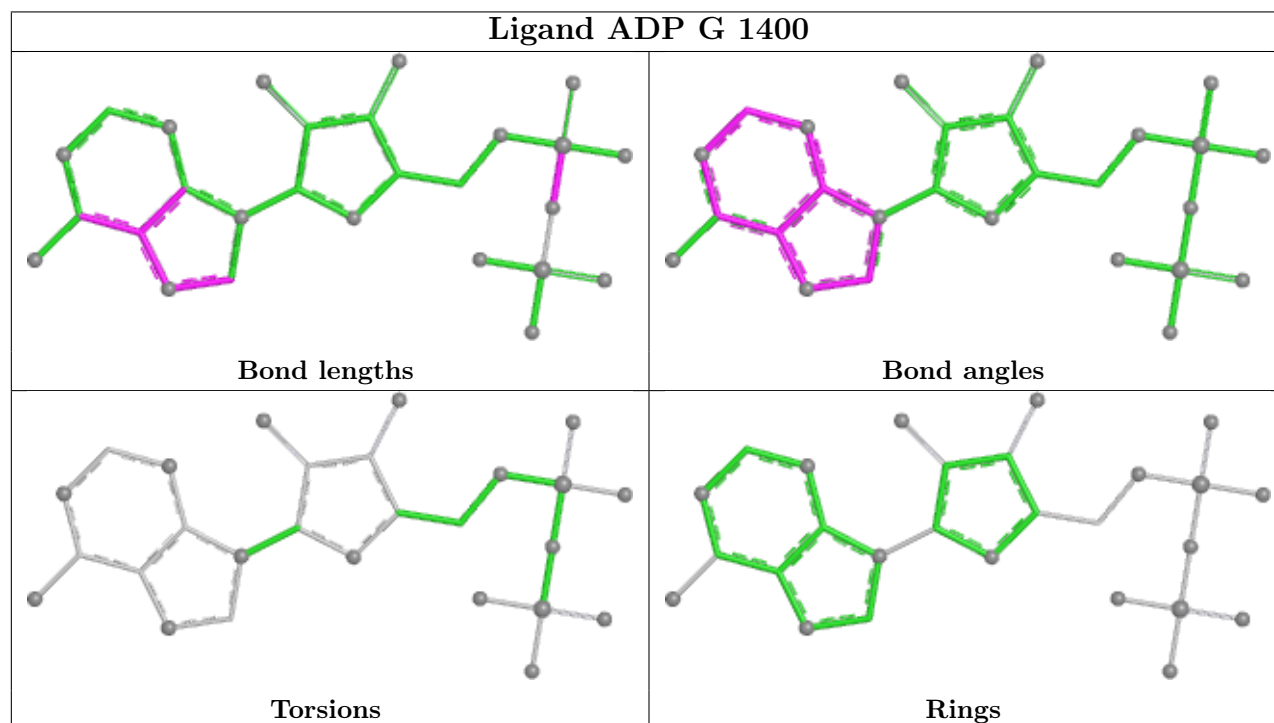
Mol	Chain	Res	Type	Atoms
3	J	1500	ADP	PB-O3A-PA-O5'

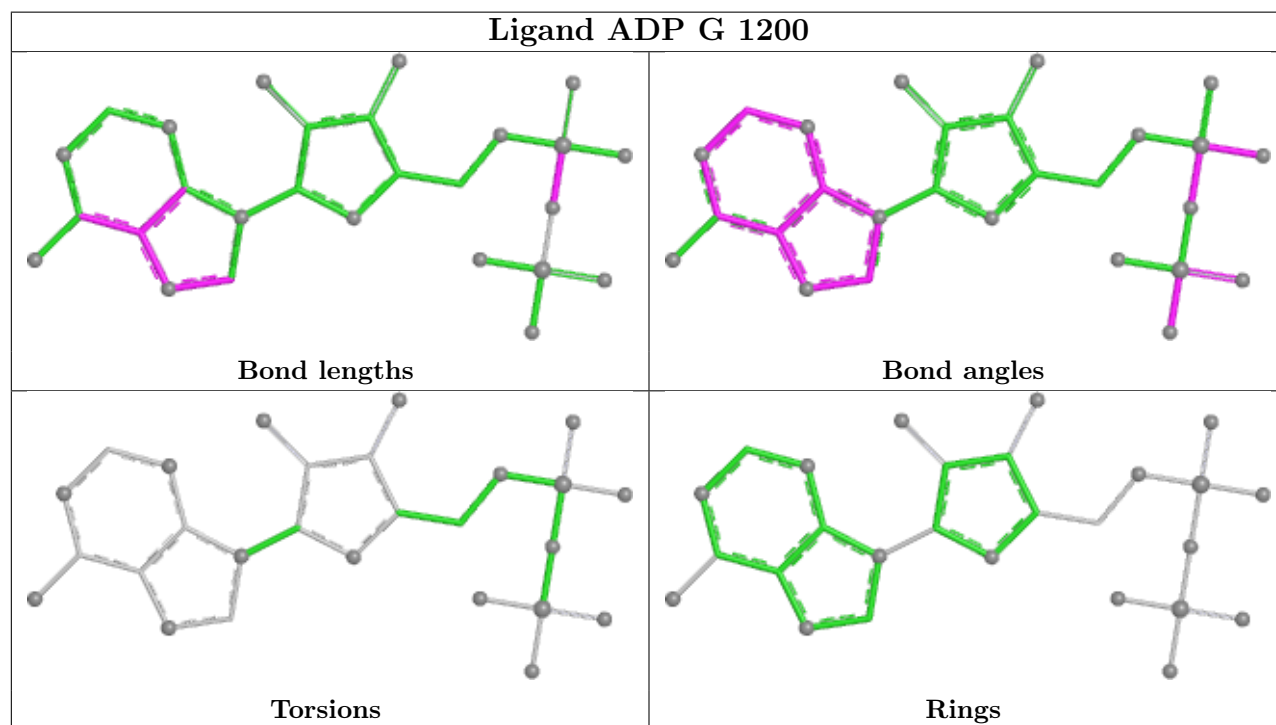
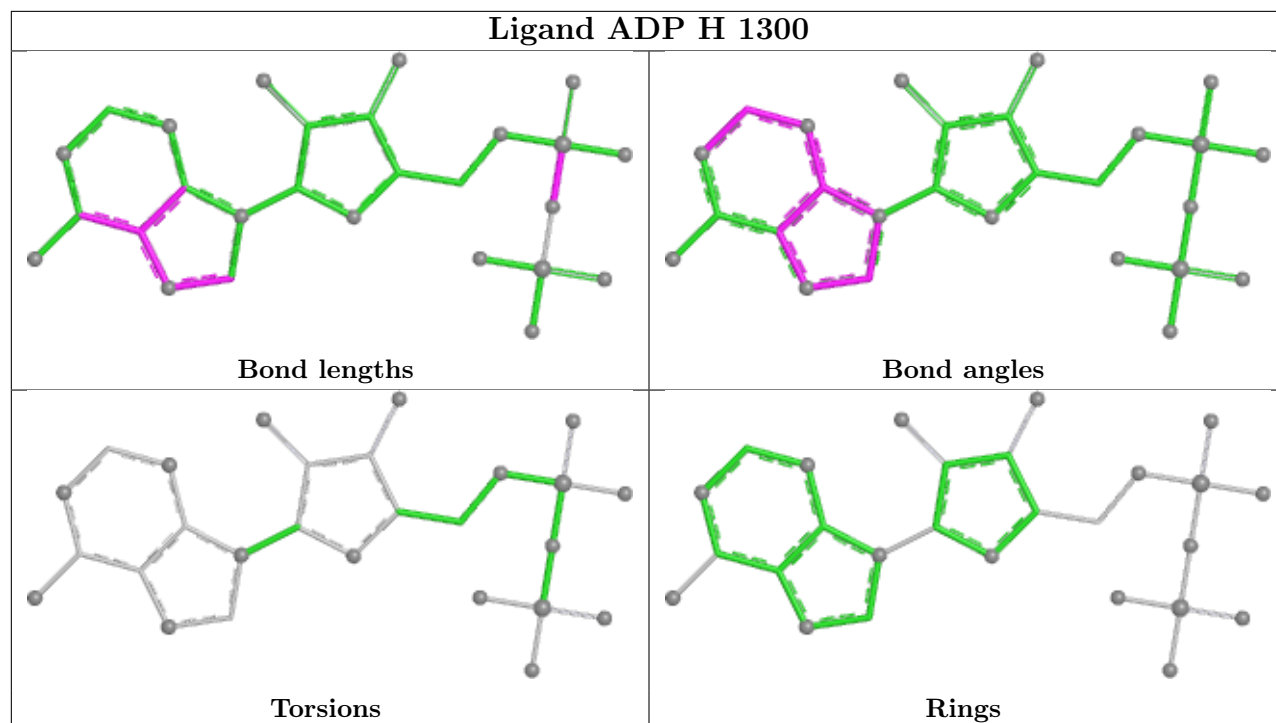
There are no ring outliers.

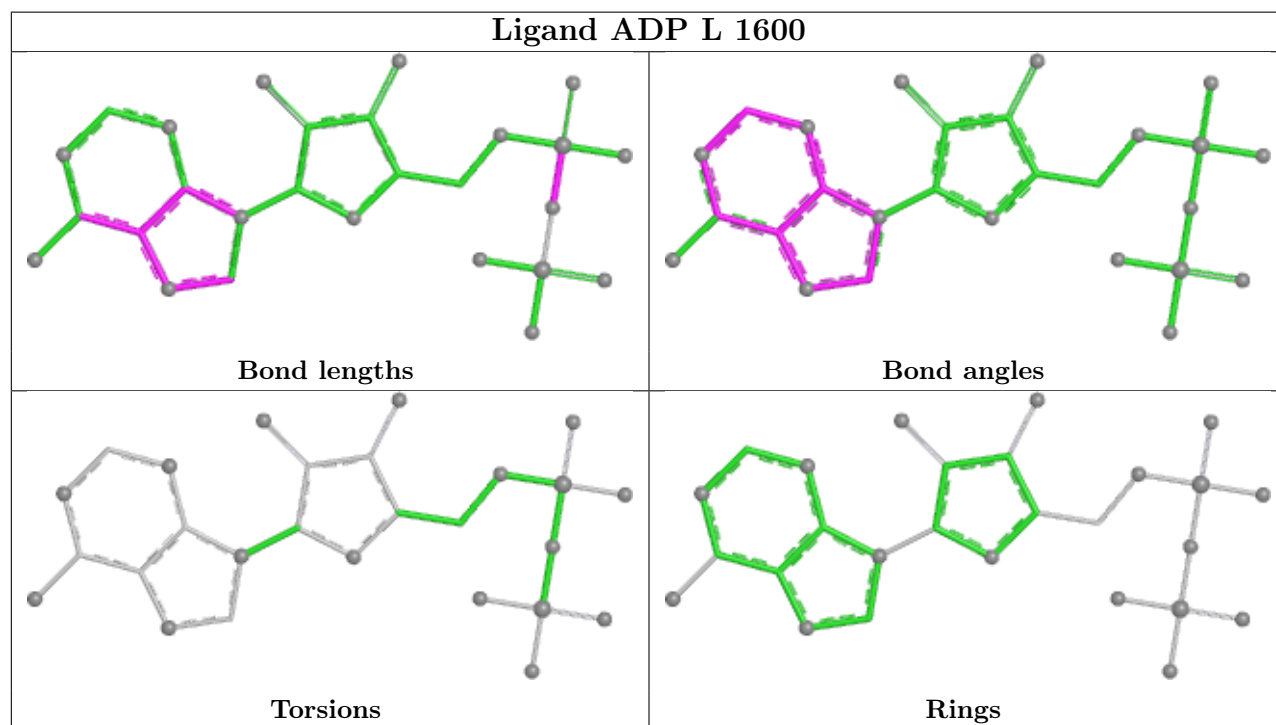
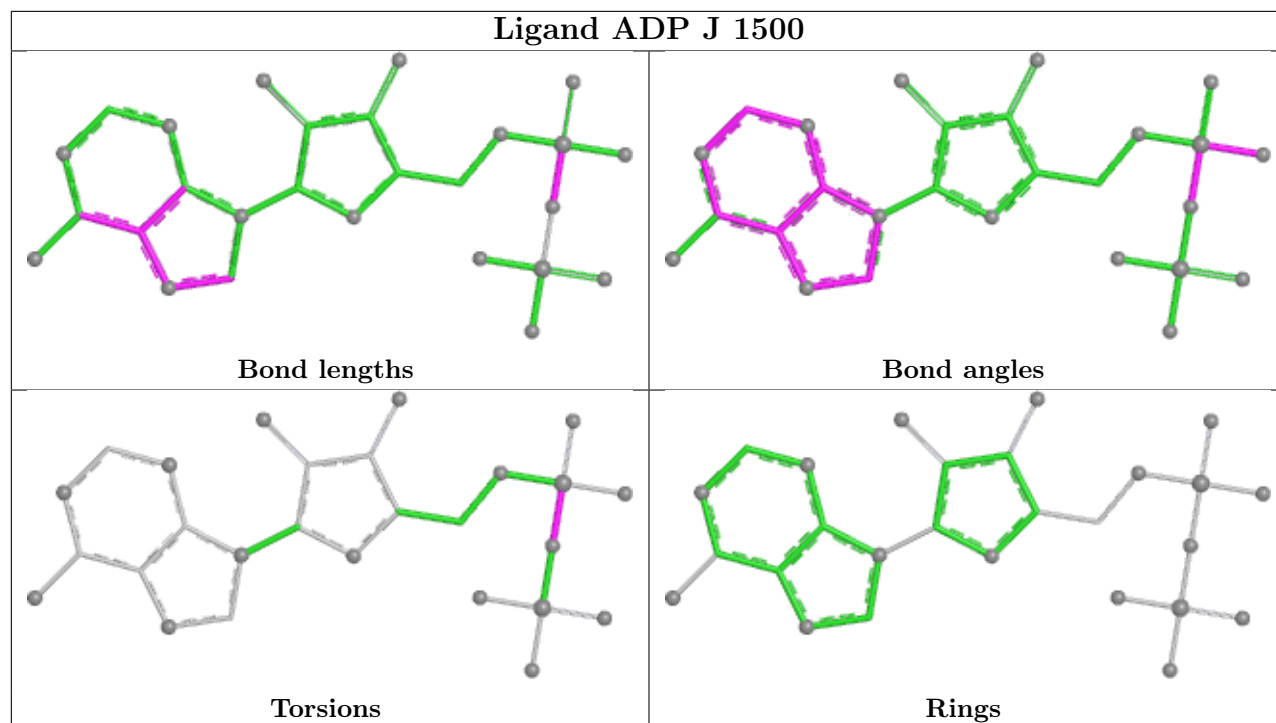
1 monomer is involved in 1 short contact:

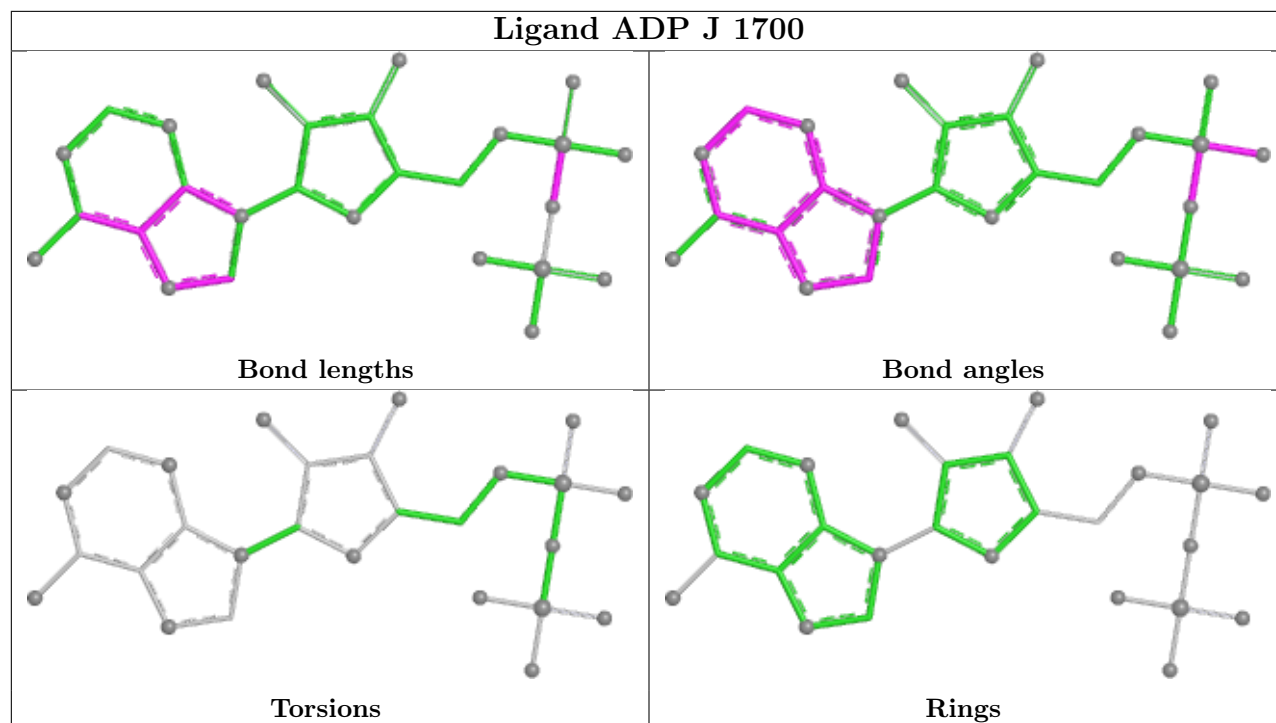
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1600	ADP	1	0

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 [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	409/415 (98%)	-0.29	1 (0%) 91 89	16, 27, 47, 86	10 (2%)
1	B	409/415 (98%)	-0.26	0 100 100	15, 27, 47, 65	11 (2%)
1	C	409/415 (98%)	-0.31	4 (0%) 79 76	15, 26, 45, 65	11 (2%)
1	D	410/415 (98%)	-0.29	7 (1%) 69 65	14, 26, 42, 82	11 (2%)
1	E	409/415 (98%)	-0.32	1 (0%) 91 89	13, 27, 49, 72	11 (2%)
1	F	409/415 (98%)	-0.29	1 (0%) 91 89	15, 27, 45, 68	11 (2%)
2	G	112/112 (100%)	-0.09	0 100 100	14, 27, 45, 56	0
2	H	112/112 (100%)	-0.06	0 100 100	16, 27, 43, 49	0
2	I	112/112 (100%)	0.30	0 100 100	12, 30, 41, 54	0
2	J	112/112 (100%)	-0.41	0 100 100	17, 28, 41, 48	0
2	K	112/112 (100%)	-0.46	0 100 100	17, 26, 43, 48	0
2	L	112/112 (100%)	-0.36	0 100 100	17, 28, 41, 50	0
All	All	3127/3162 (98%)	-0.27	14 (0%) 88 86	12, 27, 45, 86	65 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-3	HIS	3.4
1	D	406	ALA	3.1
1	C	406	ALA	3.1
1	A	75	PHE	2.9
1	C	75	PHE	2.9
1	D	88	LEU	2.5
1	D	-2	HIS	2.4
1	C	155	SER	2.3
1	C	78	ILE	2.3
1	F	310	ASP	2.1
1	E	76	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	0	HIS	2.0
1	D	254	GLY	2.0
1	D	1	HIS	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](#)

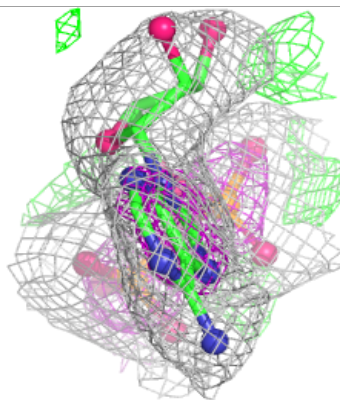
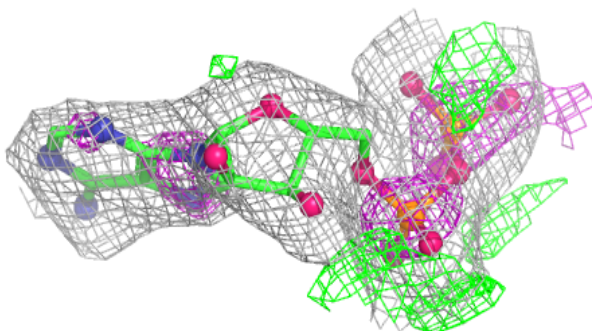
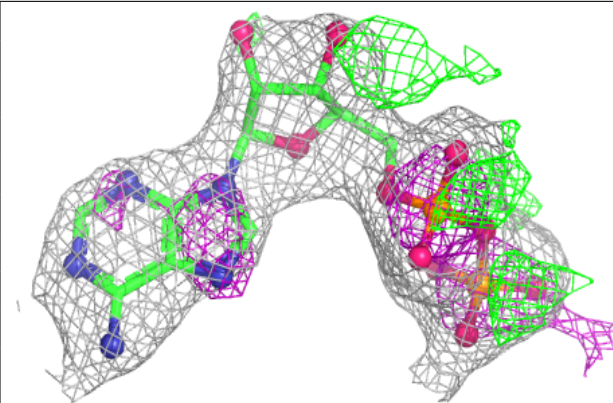
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	ADP	H	1300	27/27	0.92	0.10	2,23,30,41	0
3	ADP	G	1400	27/27	0.94	0.09	11,30,42,46	0
3	ADP	J	1500	27/27	0.96	0.06	4,17,31,37	0
3	ADP	G	1200	27/27	0.97	0.05	8,18,23,34	0
3	ADP	L	1600	27/27	0.97	0.06	10,20,31,33	0
3	ADP	J	1700	27/27	0.98	0.05	9,22,30,34	0

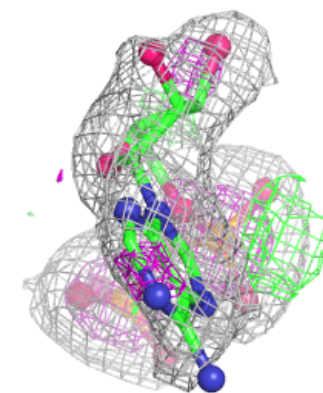
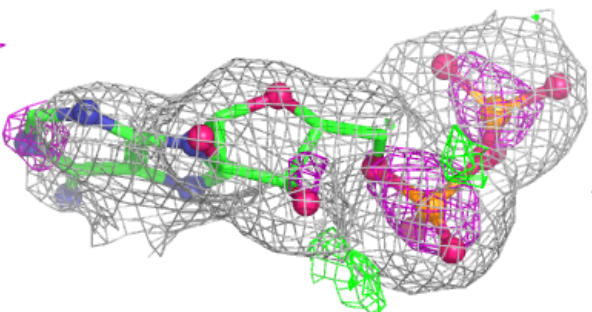
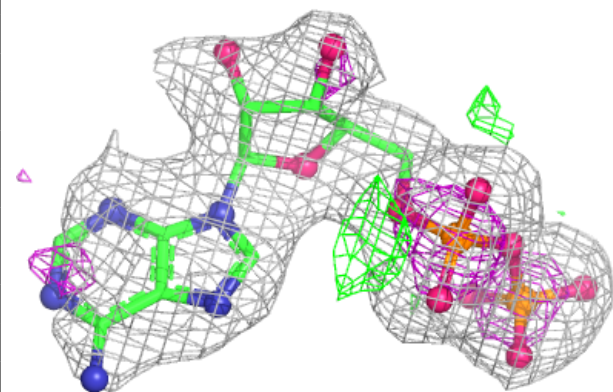
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP H 1300:

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

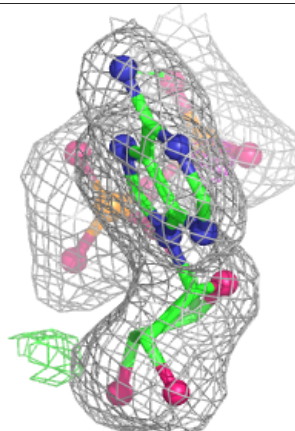
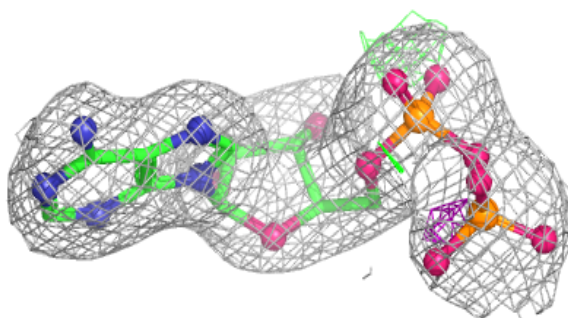
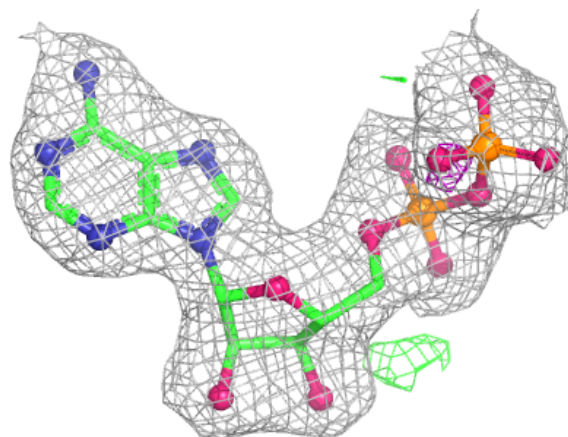
**Electron density around ADP G 1400:**

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

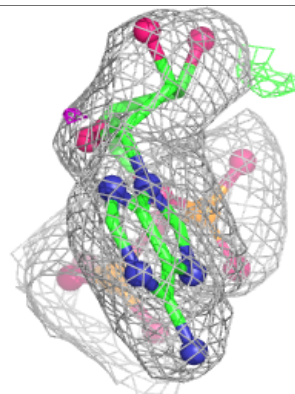
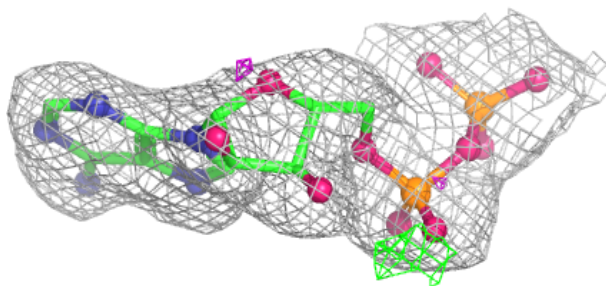
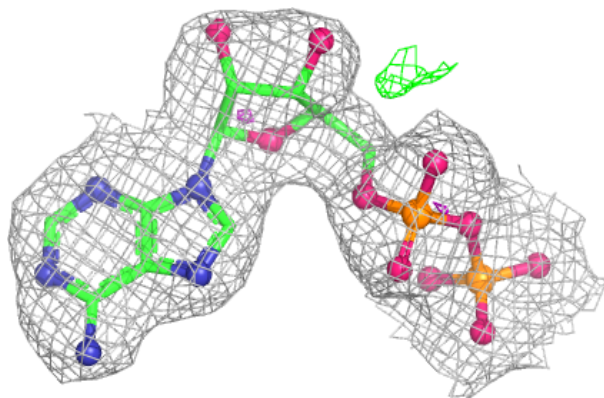


Electron density around ADP J 1500:

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

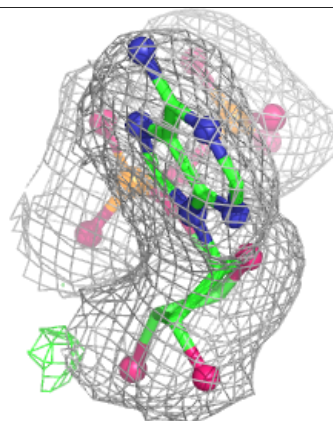
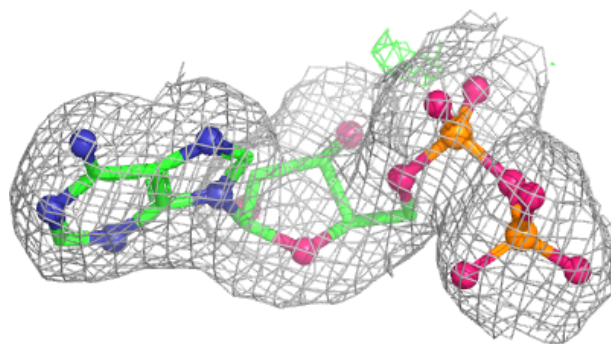
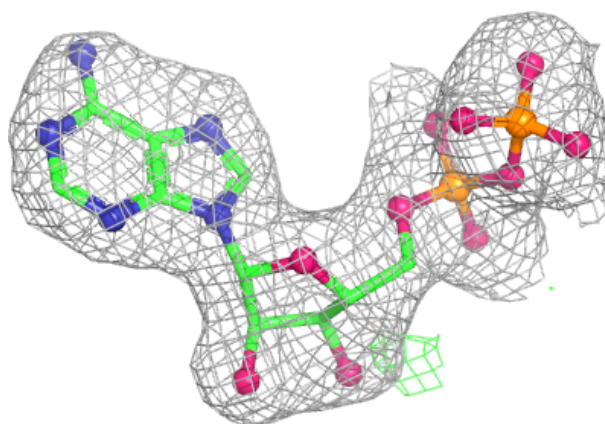
**Electron density around ADP G 1200:**

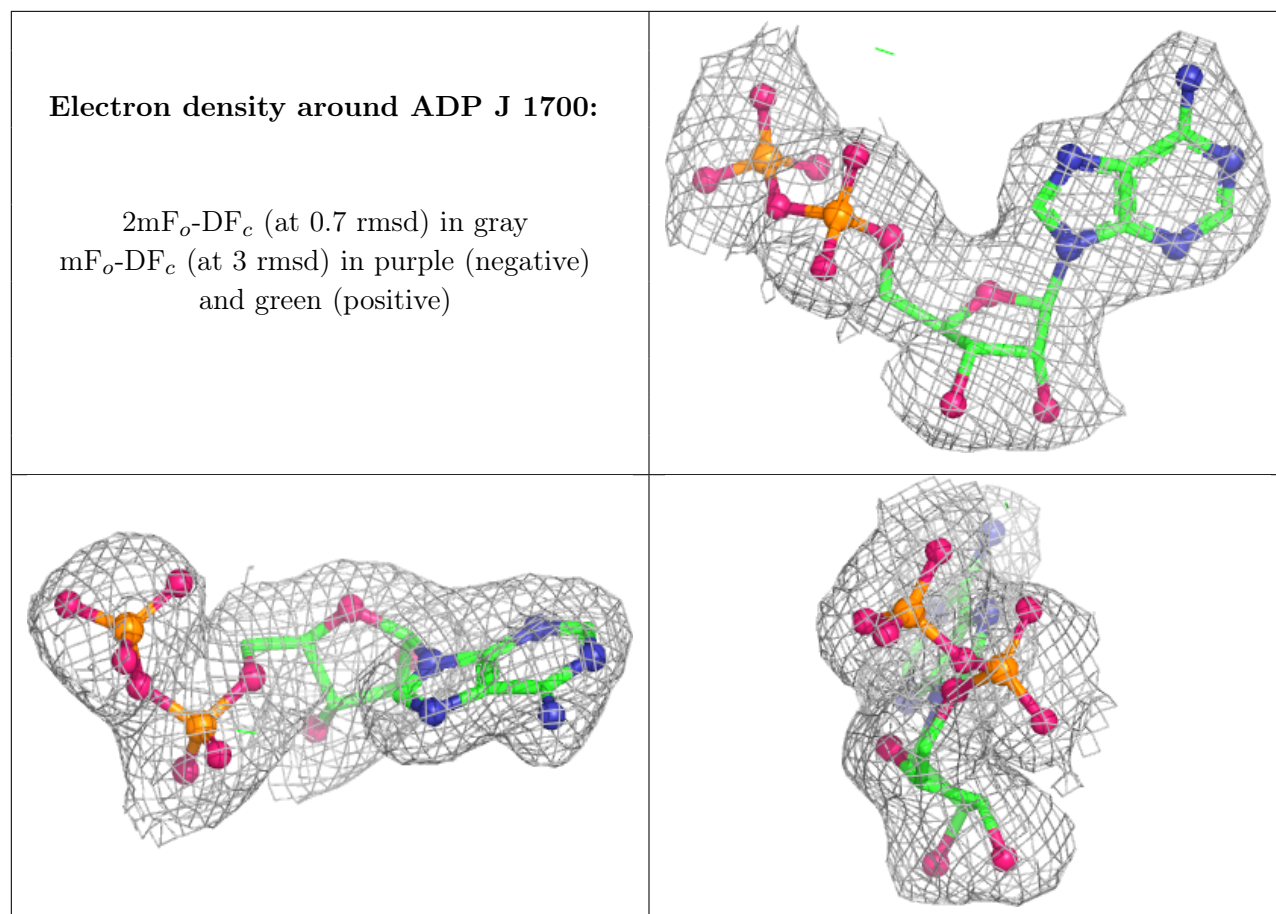
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP L 1600:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.