



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:27 PM UTC

PDB ID : 6JJ9 / pdb_00006jj9
Title : Crystal structure of OsHXK6-Glc-ATP-Mg²⁺ complex
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Deposited on : 2019-02-25
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

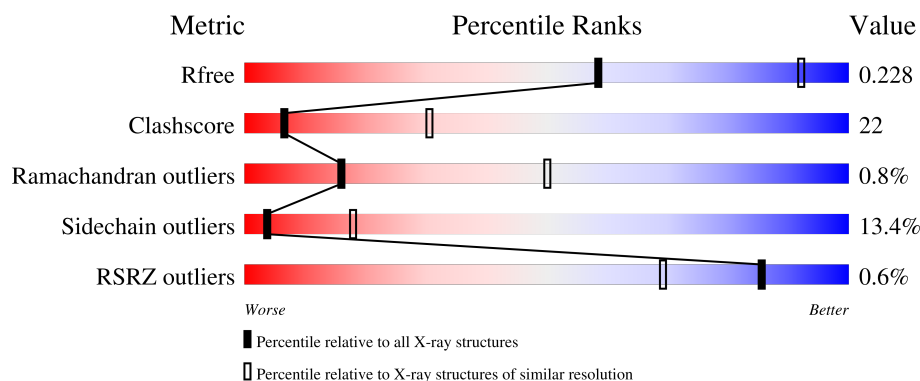
1 Overall quality at a glance

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	465	% 60% 30% 8% .
1	C	465	% 59% 30% 9% .
1	E	465	% 63% 29% 7% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10902 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 Hexokinase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	465	Total	C	N	O	S	0	0	0
			3589	2257	634	683	15			
1	A	465	Total	C	N	O	S	0	0	0
			3589	2257	634	683	15			
1	E	465	Total	C	N	O	S	0	0	0
			3589	2257	634	683	15			

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



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

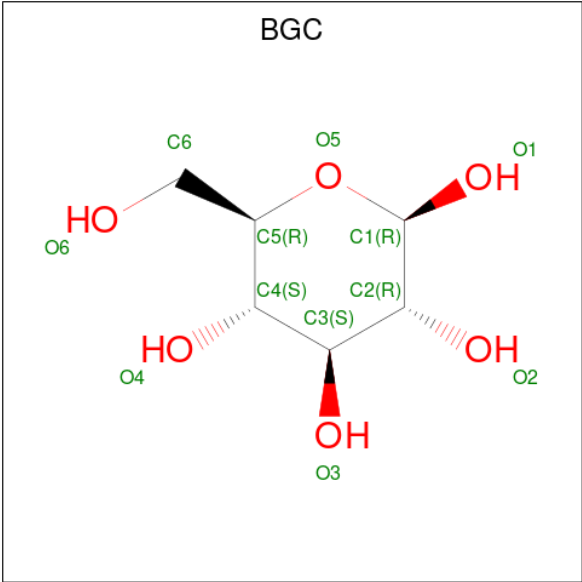


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

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

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

- Molecule 5 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).

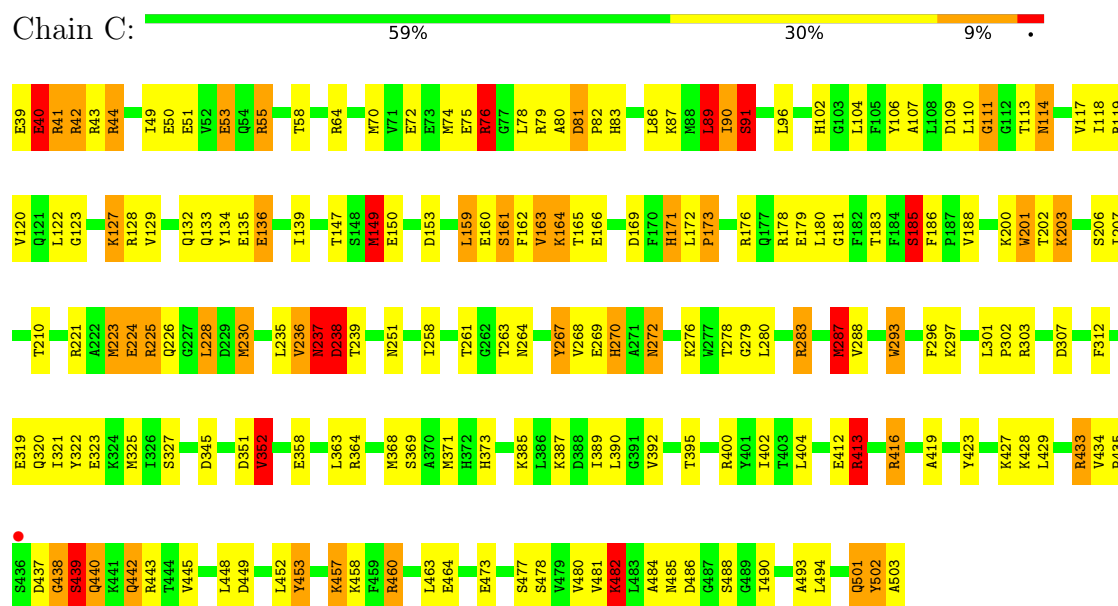


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	E	1	Total	C	O	0	0
			12	6	6		

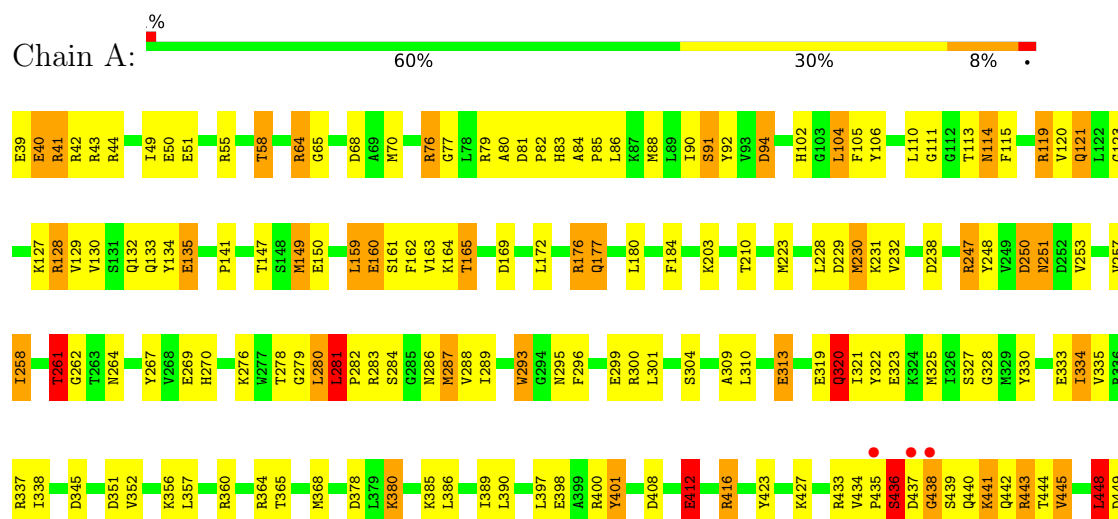
3 Residue-property plots

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: Hexokinase-6

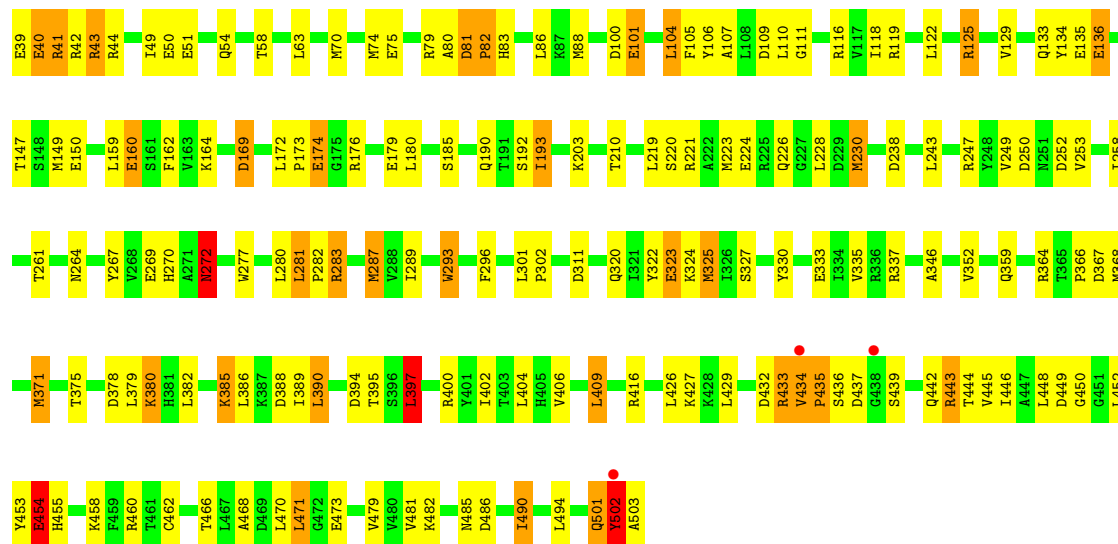


• Molecule 1: Hexokinase-6





● Molecule 1: Hexokinase-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.12Å 131.12Å 186.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.07 – 3.00 43.07 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.07-3.00) 99.1 (43.07-3.00)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.206 , 0.242 0.205 , 0.228	Depositor DCC
R_{free} test set	1989 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10902	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, PO4, MG, BGC

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	1.38	42/3652 (1.2%)	0.99	22/4936 (0.4%)
1	C	1.57	40/3652 (1.1%)	1.05	15/4936 (0.3%)
1	E	1.20	9/3652 (0.2%)	0.94	21/4936 (0.4%)
All	All	1.39	91/10956 (0.8%)	0.99	58/14808 (0.4%)

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	PHE	C-O	-8.07	1.15	1.24
1	C	460	ARG	C-O	-7.96	1.15	1.24
1	A	412	GLU	C-O	-7.89	1.15	1.24
1	C	237	ASN	CA-C	-7.71	1.42	1.52
1	C	413	ARG	C-O	-7.43	1.15	1.24
1	C	90	ILE	C-O	-7.36	1.17	1.24
1	A	287	MET	C-O	-7.29	1.15	1.23
1	A	334	ILE	C-O	-7.17	1.15	1.24
1	C	267	TYR	C-O	-6.91	1.15	1.24
1	A	257	VAL	C-O	-6.87	1.17	1.24
1	C	236	VAL	C-O	-6.84	1.16	1.23
1	E	359	GLN	C-O	-6.67	1.15	1.24
1	A	310	LEU	C-O	-6.65	1.16	1.24
1	A	445	VAL	C-O	-6.58	1.16	1.24
1	A	385	LYS	C-O	-6.44	1.16	1.24
1	A	482	LYS	C-O	-6.41	1.16	1.23
1	A	448	LEU	C-O	-6.38	1.16	1.24
1	C	238	ASP	C-O	-6.32	1.15	1.24
1	C	188	VAL	C-O	-6.29	1.17	1.24
1	C	452	LEU	C-O	-6.25	1.16	1.24
1	A	319	GLU	C-O	-6.15	1.16	1.23
1	C	200	LYS	C-O	-6.07	1.17	1.23
1	A	364	ARG	C-O	-6.04	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	VAL	C-O	-6.01	1.17	1.24
1	A	270	HIS	C-O	-5.97	1.16	1.24
1	C	81	ASP	CA-C	-5.96	1.46	1.53
1	C	114	ASN	CA-C	-5.89	1.45	1.52
1	C	320	GLN	C-O	-5.86	1.16	1.23
1	A	423	TYR	C-O	-5.85	1.17	1.24
1	A	321	ILE	C-O	-5.85	1.17	1.24
1	E	287	MET	C-O	-5.82	1.16	1.24
1	C	149	MET	C-O	-5.78	1.17	1.24
1	C	91	SER	CA-C	-5.75	1.45	1.52
1	C	55	ARG	CA-C	-5.75	1.45	1.52
1	A	267	TYR	C-O	-5.74	1.16	1.23
1	E	81	ASP	CA-C	-5.73	1.45	1.53
1	A	286	ASN	C-O	-5.73	1.16	1.23
1	C	201	TRP	C-O	-5.71	1.16	1.23
1	A	84	ALA	CA-C	-5.67	1.46	1.52
1	A	135	GLU	C-O	-5.64	1.17	1.24
1	C	64	ARG	C-O	-5.60	1.17	1.24
1	A	463	LEU	C-O	-5.59	1.17	1.24
1	C	368	MET	C-O	-5.55	1.17	1.24
1	A	360	ARG	C-O	-5.52	1.17	1.23
1	C	114	ASN	C-O	-5.49	1.17	1.23
1	E	323	GLU	C-O	-5.48	1.17	1.24
1	C	237	ASN	C-O	-5.42	1.17	1.24
1	C	50	GLU	C-O	-5.41	1.17	1.24
1	E	382	LEU	C-O	-5.40	1.17	1.24
1	C	453	TYR	C-O	-5.39	1.17	1.24
1	C	416	ARG	C-O	-5.38	1.17	1.23
1	A	114	ASN	C-O	-5.38	1.17	1.23
1	A	401	TYR	C-O	-5.37	1.17	1.24
1	C	109	ASP	C-O	-5.37	1.18	1.24
1	C	268	VAL	C-O	-5.36	1.18	1.24
1	A	177	GLN	C-O	-5.36	1.17	1.24
1	C	303	ARG	C-O	-5.36	1.17	1.23
1	C	482	LYS	C-O	-5.35	1.17	1.23
1	C	364	ARG	C-O	-5.34	1.16	1.23
1	A	320	GLN	C-O	-5.33	1.16	1.23
1	A	457	LYS	C-O	-5.32	1.17	1.24
1	A	76	ARG	C-O	-5.32	1.17	1.24
1	E	280	LEU	C-O	-5.30	1.17	1.23
1	A	115	PHE	C-O	-5.29	1.17	1.23
1	A	55	ARG	C-O	-5.28	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	ARG	C-O	-5.28	1.17	1.24
1	A	444	THR	C-O	-5.28	1.17	1.24
1	E	389	ILE	C-O	-5.25	1.17	1.24
1	A	119	ARG	C-O	-5.22	1.17	1.23
1	A	456	TYR	C-O	-5.22	1.17	1.23
1	C	352	VAL	C-O	-5.22	1.17	1.24
1	A	70	MET	C-O	-5.22	1.18	1.24
1	A	111	GLY	C-O	-5.20	1.18	1.24
1	C	369	SER	C-O	-5.20	1.18	1.24
1	E	371	MET	N-CA	-5.18	1.40	1.46
1	A	250	ASP	C-O	-5.17	1.17	1.24
1	C	287	MET	C-O	-5.17	1.17	1.23
1	A	368	MET	C-O	-5.15	1.17	1.24
1	A	64	ARG	C-O	-5.14	1.18	1.24
1	C	321	ILE	C-O	-5.13	1.18	1.24
1	C	76	ARG	C-O	-5.13	1.18	1.24
1	A	453	TYR	C-O	-5.12	1.18	1.24
1	E	160	GLU	C-O	-5.12	1.18	1.24
1	C	319	GLU	CA-C	-5.10	1.46	1.52
1	C	72	GLU	C-O	-5.07	1.18	1.24
1	A	269	GLU	C-O	-5.06	1.17	1.23
1	A	278	THR	CA-C	-5.05	1.46	1.52
1	C	206	SER	C-O	-5.04	1.17	1.24
1	C	270	HIS	CA-C	-5.02	1.46	1.52
1	C	490	ILE	C-O	-5.02	1.17	1.24
1	A	258	ILE	C-O	-5.01	1.19	1.24

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	THR	N-CA-C	-12.86	89.59	109.52
1	C	40	GLU	N-CA-C	-11.92	97.28	112.90
1	E	471	LEU	N-CA-C	-9.56	97.65	110.55
1	E	40	GLU	N-CA-C	-8.57	101.88	111.14
1	C	181	GLY	N-CA-C	-8.51	97.70	110.71
1	A	280	LEU	N-CA-C	8.38	123.08	109.76
1	A	177	GLN	CA-C-N	7.99	132.17	120.90
1	A	177	GLN	C-N-CA	7.99	132.17	120.90
1	A	443	ARG	N-CA-C	-7.39	97.19	109.46
1	C	239	THR	N-CA-C	-7.31	103.32	112.90
1	E	434	VAL	C-N-CD	6.92	135.83	120.60
1	C	321	ILE	N-CA-C	6.89	117.60	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	GLU	N-CA-C	-6.83	103.90	111.82
1	A	441	LYS	N-CA-C	-6.62	102.26	110.41
1	C	89	LEU	N-CA-C	6.61	120.28	109.76
1	A	251	ASN	N-CA-C	6.50	119.36	111.82
1	C	81	ASP	N-CA-C	-6.34	101.34	110.08
1	A	501	GLN	N-CA-C	6.30	121.09	113.41
1	E	502	TYR	CA-CB-CG	6.21	125.08	113.90
1	A	457	LYS	N-CA-C	6.20	118.58	111.02
1	A	437	ASP	N-CA-C	-6.19	105.73	113.28
1	A	473	GLU	N-CA-C	-6.18	104.54	111.28
1	C	428	LYS	N-CA-C	-6.13	103.93	112.45
1	E	379	LEU	CA-C-N	6.11	128.46	120.28
1	E	379	LEU	C-N-CA	6.11	128.46	120.28
1	E	501	GLN	N-CA-C	6.06	120.77	112.04
1	E	382	LEU	N-CA-C	-5.98	104.84	111.36
1	C	171	HIS	N-CA-C	5.79	118.93	108.69
1	A	279	GLY	CA-C-N	5.63	129.55	121.50
1	A	279	GLY	C-N-CA	5.63	129.55	121.50
1	C	438	GLY	N-CA-C	-5.51	97.33	113.30
1	C	203	LYS	N-CA-C	5.50	118.92	111.17
1	E	502	TYR	CB-CA-C	5.47	120.50	110.10
1	E	502	TYR	N-CA-CB	5.44	119.75	110.50
1	A	442	GLN	N-CA-C	-5.42	101.73	110.14
1	E	82	PRO	CA-N-CD	-5.40	104.44	112.00
1	E	385	LYS	N-CA-C	-5.40	104.95	112.45
1	A	281	LEU	N-CA-C	5.37	121.67	109.81
1	E	272	ASN	N-CA-C	-5.35	106.80	113.38
1	A	438	GLY	N-CA-C	-5.32	106.20	112.64
1	E	380	LYS	CB-CA-C	-5.29	102.01	110.79
1	A	81	ASP	CA-C-N	-5.25	113.89	120.51
1	A	81	ASP	C-N-CA	-5.25	113.89	120.51
1	A	299	GLU	N-CA-C	-5.22	106.96	113.38
1	C	502	TYR	N-CA-C	5.20	125.56	111.00
1	A	338	ILE	N-CA-C	-5.20	105.78	110.82
1	E	454	GLU	N-CA-C	5.18	117.83	111.82
1	E	389	ILE	N-CA-C	5.16	115.93	110.72
1	C	111	GLY	N-CA-C	-5.16	98.35	113.30
1	A	261	THR	CB-CA-C	5.15	119.61	110.85
1	C	501	GLN	N-CA-C	5.08	119.51	112.45
1	E	388	ASP	CA-C-N	5.08	127.63	120.42
1	E	388	ASP	C-N-CA	5.08	127.63	120.42
1	E	389	ILE	CA-C-N	-5.02	113.58	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	389	ILE	C-N-CA	-5.02	113.58	122.26
1	E	397	LEU	N-CA-C	-5.00	106.02	111.82
1	C	439	SER	N-CA-C	5.00	121.45	110.80
1	A	128	ARG	N-CA-C	5.00	116.53	108.08

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	3589	0	3582	140	2
1	C	3589	0	3581	181	3
1	E	3589	0	3575	152	0
2	A	27	0	12	3	0
2	C	27	0	12	1	0
2	E	27	0	12	3	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	12	0	11	4	0
5	C	12	0	11	5	0
5	E	12	0	11	2	0
All	All	10902	0	10807	471	3

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 22.

All (471) 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:C:176:ARG:HG2	1:C:503:ALA:CB	1.39	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:PRO:HG2	1:E:436:SER:CB	1.55	1.36
1:C:166:GLU:OE1	1:C:178:ARG:NH1	1.57	1.33
1:A:160:GLU:OE2	1:A:164:LYS:HE3	1.27	1.33
1:A:176:ARG:CD	1:A:503:ALA:HA	1.56	1.32
1:A:176:ARG:HD3	1:A:503:ALA:CA	1.58	1.31
1:C:176:ARG:CG	1:C:503:ALA:HB1	1.62	1.29
1:E:436:SER:OG	1:E:437:ASP:OD2	1.53	1.25
1:E:119:ARG:NH1	1:E:133:GLN:OE1	1.71	1.22
1:A:119:ARG:NH1	1:A:133:GLN:OE1	1.82	1.13
1:E:435:PRO:HB2	1:E:436:SER:HA	1.20	1.12
1:E:367:ASP:OD1	1:E:385:LYS:NZ	1.83	1.12
1:E:435:PRO:CB	1:E:436:SER:HA	1.79	1.11
1:C:435:PRO:HG3	1:C:440:GLN:O	1.51	1.10
1:E:433:ARG:HB3	1:E:433:ARG:HH21	1.16	1.09
1:C:78:LEU:O	1:C:276:LYS:HG2	1.55	1.06
1:A:231:LYS:NZ	1:A:501:GLN:HE21	1.52	1.06
1:C:42:ARG:HB2	1:C:42:ARG:HH21	1.14	1.06
1:C:433:ARG:HH21	1:C:433:ARG:HB3	1.16	1.05
1:C:173:PRO:HB2	1:C:176:ARG:HD2	1.06	1.05
1:C:180:LEU:HD22	1:C:223:MET:HE1	1.39	1.04
1:C:437:ASP:HB2	1:C:439:SER:CB	1.89	1.02
1:E:409:LEU:HD12	1:E:409:LEU:H	1.24	1.01
1:A:91:SER:OG	1:A:288:VAL:O	1.80	1.00
1:A:261:THR:O	1:A:327:SER:OG	1.78	1.00
1:E:435:PRO:HG2	1:E:436:SER:CA	1.92	0.99
1:C:119:ARG:NH1	1:C:133:GLN:OE1	1.96	0.98
1:C:287:MET:HE2	1:C:287:MET:HA	1.43	0.98
1:E:435:PRO:HG2	1:E:436:SER:HB2	1.44	0.97
1:C:51:GLU:O	1:C:55:ARG:HG2	1.64	0.97
1:C:437:ASP:HB2	1:C:439:SER:HB2	1.46	0.97
1:E:435:PRO:HG2	1:E:436:SER:HB3	1.47	0.96
1:E:436:SER:HB2	1:E:437:ASP:HA	1.48	0.96
1:C:173:PRO:CB	1:C:176:ARG:HD2	1.96	0.95
1:A:231:LYS:HZ2	1:A:501:GLN:HE21	1.14	0.94
1:A:120:VAL:HG12	1:A:132:GLN:HG3	1.50	0.94
1:C:173:PRO:HB2	1:C:176:ARG:CD	1.99	0.93
1:E:281:LEU:HD22	1:E:282:PRO:HD2	1.51	0.92
1:C:434:VAL:HG12	1:C:435:PRO:HD2	1.49	0.92
1:A:90:ILE:CG2	1:A:287:MET:HE3	1.98	0.91
1:E:435:PRO:CG	1:E:436:SER:HA	2.01	0.91
1:C:280:LEU:H	1:C:280:LEU:HD23	1.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:HB2	1:C:42:ARG:NH2	1.86	0.91
1:C:283:ARG:H	1:C:283:ARG:HD3	1.33	0.90
1:E:283:ARG:H	1:E:283:ARG:HD3	1.32	0.90
1:A:231:LYS:NZ	1:A:501:GLN:NE2	2.21	0.88
1:E:436:SER:CB	1:E:437:ASP:HA	1.98	0.88
1:E:435:PRO:CG	1:E:436:SER:CB	2.49	0.88
1:E:406:VAL:HA	1:E:409:LEU:HD13	1.54	0.87
1:E:435:PRO:HB2	1:E:436:SER:CA	2.04	0.87
1:E:433:ARG:HH21	1:E:433:ARG:CB	1.88	0.87
1:C:437:ASP:H	1:C:438:GLY:C	1.83	0.86
1:E:179:GLU:OE2	1:E:501:GLN:HG3	1.75	0.86
1:C:114:ASN:HD22	1:C:136:GLU:CD	1.82	0.86
1:A:160:GLU:OE2	1:A:164:LYS:CE	2.20	0.86
1:C:51:GLU:HG2	1:C:55:ARG:HD3	1.54	0.86
1:C:423:TYR:O	1:C:427:LYS:HG3	1.76	0.85
1:E:435:PRO:CB	1:E:436:SER:CA	2.54	0.85
1:C:434:VAL:CG1	1:C:435:PRO:HD2	2.05	0.85
1:E:435:PRO:CG	1:E:436:SER:CA	2.54	0.84
1:A:261:THR:CG2	2:A:601:ADP:O3B	2.26	0.83
1:E:281:LEU:HD22	1:E:282:PRO:CD	2.07	0.83
1:C:176:ARG:CG	1:C:503:ALA:CB	2.34	0.83
1:A:41:ARG:HG3	1:A:41:ARG:HH11	1.42	0.83
1:A:90:ILE:CG2	1:A:287:MET:CE	2.56	0.83
1:A:501:GLN:N	1:A:502:TYR:HA	1.91	0.83
1:A:44:ARG:HD3	1:A:345:ASP:O	1.79	0.82
1:A:501:GLN:H	1:A:502:TYR:HA	1.44	0.82
1:C:433:ARG:HH21	1:C:433:ARG:CB	1.92	0.82
1:C:433:ARG:HB3	1:C:433:ARG:NH2	1.94	0.82
1:C:180:LEU:CD2	1:C:223:MET:HE1	2.09	0.82
1:E:320:GLN:O	1:E:324:LYS:HG3	1.79	0.82
1:C:76:ARG:HG2	1:C:76:ARG:HH11	1.45	0.82
1:C:91:SER:OG	1:C:288:VAL:O	1.96	0.81
1:A:90:ILE:HG22	1:A:287:MET:HE3	1.61	0.81
1:A:104:LEU:HB2	1:A:121:GLN:OE1	1.79	0.81
1:A:128:ARG:NH2	1:A:248:TYR:O	2.13	0.81
1:C:435:PRO:CG	1:C:440:GLN:O	2.28	0.81
1:C:437:ASP:HB2	1:C:439:SER:HB3	1.61	0.81
1:A:247:ARG:NH2	1:A:253:VAL:O	2.14	0.81
1:E:180:LEU:HD22	1:E:223:MET:HE1	1.61	0.80
1:A:39:GLU:HG3	1:A:40:GLU:H	1.46	0.79
1:C:179:GLU:OE2	1:C:501:GLN:HG3	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ARG:HG2	1:C:503:ALA:HB2	1.62	0.79
1:A:90:ILE:HG23	1:A:287:MET:HE3	1.66	0.78
1:E:43:ARG:HG3	1:E:44:ARG:N	1.99	0.78
1:A:58:THR:O	1:A:416:ARG:NH1	2.17	0.77
1:C:439:SER:OG	1:C:440:GLN:N	2.17	0.77
1:C:269:GLU:HG3	1:C:270:HIS:N	1.98	0.77
1:A:231:LYS:HZ2	1:A:501:GLN:NE2	1.81	0.77
1:A:448:LEU:HD13	1:A:481:VAL:HG13	1.66	0.77
1:C:448:LEU:HD13	1:C:481:VAL:HG13	1.67	0.76
1:C:114:ASN:ND2	1:C:136:GLU:CD	2.43	0.76
1:C:437:ASP:CB	1:C:439:SER:HB2	2.15	0.76
1:C:437:ASP:N	1:C:438:GLY:O	2.17	0.75
1:E:261:THR:O	1:E:327:SER:OG	2.04	0.75
1:E:250:ASP:OD1	1:E:443:ARG:NH2	2.18	0.75
1:C:76:ARG:HG2	1:C:76:ARG:NH1	1.98	0.75
1:E:371:MET:CE	1:E:386:LEU:HG	2.16	0.75
1:E:471:LEU:HD11	1:E:479:VAL:HG21	1.67	0.74
1:A:231:LYS:HZ3	1:A:501:GLN:HE21	1.33	0.74
1:C:280:LEU:H	1:C:280:LEU:CD2	1.98	0.74
1:E:180:LEU:CD2	1:E:223:MET:HE1	2.17	0.74
1:C:434:VAL:HG12	1:C:435:PRO:CD	2.17	0.74
1:A:39:GLU:HG3	1:A:40:GLU:N	2.01	0.74
1:A:434:VAL:HG21	1:A:474:GLU:OE2	1.87	0.74
1:C:287:MET:HA	1:C:287:MET:CE	2.16	0.74
1:C:261:THR:O	1:C:327:SER:OG	2.06	0.73
1:A:261:THR:HG23	2:A:601:ADP:O3B	1.87	0.73
1:C:110:LEU:O	1:C:185:SER:OG	2.05	0.73
1:E:409:LEU:H	1:E:409:LEU:CD1	2.01	0.73
1:C:283:ARG:H	1:C:283:ARG:CD	1.97	0.72
1:E:448:LEU:HD13	1:E:481:VAL:HG13	1.71	0.72
1:A:250:ASP:OD1	1:A:443:ARG:NH2	2.23	0.71
1:E:79:ARG:O	1:E:80:ALA:HB3	1.90	0.71
1:C:301:LEU:HD13	1:C:325:MET:HE1	1.73	0.71
1:E:409:LEU:HD12	1:E:409:LEU:N	2.03	0.71
1:C:437:ASP:H	1:C:438:GLY:CA	2.03	0.71
1:E:100:ASP:OD2	1:E:125:ARG:HD3	1.90	0.71
1:A:41:ARG:HH11	1:A:41:ARG:CG	2.04	0.70
1:E:160:GLU:OE2	1:E:164:LYS:HE3	1.90	0.70
1:A:64:ARG:NH1	1:A:470:LEU:O	2.24	0.70
1:A:90:ILE:HG23	1:A:287:MET:CE	2.20	0.70
1:A:323:GLU:OE2	5:A:604:BGC:O1	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:THR:O	1:C:416:ARG:NH1	2.24	0.69
1:A:180:LEU:HD22	1:A:223:MET:HE1	1.74	0.69
1:C:176:ARG:HG2	1:C:503:ALA:HB1	0.70	0.69
1:E:433:ARG:HB3	1:E:433:ARG:NH2	1.99	0.69
1:E:193:ILE:HG13	1:E:193:ILE:O	1.90	0.69
1:E:435:PRO:CG	1:E:436:SER:HB2	2.18	0.69
1:A:160:GLU:CD	1:A:164:LYS:HE3	2.14	0.69
1:C:269:GLU:HG3	1:C:270:HIS:H	1.56	0.69
1:A:438:GLY:N	1:A:439:SER:HA	2.08	0.69
1:C:236:VAL:C	1:C:237:ASN:O	2.29	0.68
1:A:176:ARG:HD3	1:A:503:ALA:HA	0.74	0.68
1:C:501:GLN:N	1:C:502:TYR:HA	2.08	0.68
1:C:437:ASP:N	1:C:438:GLY:CA	2.56	0.67
1:E:335:VAL:HG21	1:E:368:MET:HE3	1.77	0.67
1:E:203:LYS:NZ	5:E:604:BGC:O6	2.28	0.67
1:A:68:ASP:OD2	1:A:427:LYS:NZ	2.27	0.67
1:E:301:LEU:HB3	1:E:325:MET:HE1	1.75	0.67
1:E:436:SER:CB	1:E:437:ASP:CA	2.73	0.67
1:E:147:THR:HB	1:E:150:GLU:HG3	1.75	0.66
1:C:147:THR:HG22	1:C:149:MET:H	1.60	0.66
1:E:501:GLN:N	1:E:502:TYR:HA	2.11	0.66
1:C:301:LEU:HD13	1:C:325:MET:CE	2.26	0.66
1:C:238:ASP:OD1	5:C:604:BGC:O4	2.06	0.65
1:E:311:ASP:OD1	1:E:324:LYS:NZ	2.29	0.65
1:C:437:ASP:N	1:C:438:GLY:C	2.54	0.65
1:A:378:ASP:OD1	1:A:380:LYS:NZ	2.30	0.65
1:C:44:ARG:HG2	1:C:345:ASP:O	1.96	0.65
1:C:120:VAL:HG12	1:C:132:GLN:HG3	1.79	0.64
1:C:437:ASP:N	1:C:438:GLY:HA2	2.13	0.64
1:A:330:TYR:O	1:A:334:ILE:HG13	1.97	0.64
1:A:231:LYS:HZ3	1:A:501:GLN:NE2	1.93	0.63
1:A:77:GLY:O	1:A:276:LYS:HE2	1.98	0.63
1:E:453:TYR:CE1	1:E:460:ARG:HG3	2.34	0.62
1:C:49:ILE:O	1:C:53:GLU:CG	2.48	0.62
1:E:473:GLU:OE1	1:E:473:GLU:N	2.25	0.62
1:A:258:ILE:HD13	1:A:449:ASP:HB3	1.81	0.61
1:A:436:SER:O	1:A:439:SER:HB2	2.00	0.61
1:C:49:ILE:O	1:C:53:GLU:HG3	2.00	0.61
1:E:283:ARG:HD3	1:E:283:ARG:N	2.10	0.61
1:E:335:VAL:CG2	1:E:368:MET:HE3	2.31	0.61
1:E:101:GLU:HG3	1:E:494:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PRO:O	1:A:83:HIS:HB2	2.01	0.61
1:A:90:ILE:HG22	1:A:287:MET:CE	2.24	0.61
1:A:282:PRO:O	1:A:283:ARG:C	2.39	0.61
1:C:40:GLU:O	1:C:42:ARG:N	2.34	0.60
1:C:438:GLY:O	1:C:439:SER:HB3	2.01	0.60
1:C:76:ARG:HH11	1:C:76:ARG:CG	2.13	0.60
1:C:237:ASN:CG	1:C:238:ASP:H	2.09	0.60
1:E:58:THR:O	1:E:416:ARG:NH1	2.34	0.60
1:A:238:ASP:OD2	5:A:604:BGC:H6C1	2.01	0.60
1:E:434:VAL:HG23	1:E:434:VAL:O	2.01	0.60
1:C:129:VAL:HG13	1:C:129:VAL:O	2.00	0.60
1:C:49:ILE:HD11	1:C:402:ILE:HG23	1.84	0.59
1:E:261:THR:OG1	2:E:601:ADP:O1B	2.12	0.59
1:C:40:GLU:O	1:C:41:ARG:C	2.42	0.59
1:C:373:HIS:NE2	1:C:458:LYS:HG3	2.18	0.59
1:E:106:TYR:HB2	1:E:230:MET:CE	2.32	0.59
1:C:264:ASN:CB	5:C:604:BGC:H5	2.32	0.59
1:C:351:ASP:O	1:C:352:VAL:HG12	2.03	0.59
1:C:87:LYS:HB3	1:C:89:LEU:HD21	1.84	0.59
1:C:161:SER:O	1:C:165:THR:HG23	2.02	0.59
1:A:92:TYR:HA	1:A:287:MET:HE1	1.85	0.59
1:C:159:LEU:O	1:C:163:VAL:HG13	2.03	0.58
1:E:501:GLN:H	1:E:502:TYR:HA	1.68	0.58
1:A:301:LEU:HB3	1:A:325:MET:HE1	1.84	0.58
1:C:147:THR:HB	1:C:150:GLU:HG3	1.84	0.58
1:C:264:ASN:HB2	5:C:604:BGC:H5	1.84	0.58
1:A:162:PHE:O	1:A:165:THR:CG2	2.52	0.58
1:E:40:GLU:O	1:E:41:ARG:C	2.45	0.58
1:C:228:LEU:HD22	1:C:230:MET:HG3	1.85	0.57
1:C:51:GLU:CG	1:C:55:ARG:HD3	2.30	0.57
1:C:113:THR:O	1:C:113:THR:HG22	2.05	0.57
1:A:147:THR:HB	1:A:150:GLU:HG3	1.86	0.57
1:C:224:GLU:C	1:C:226:GLN:H	2.12	0.57
1:C:412:GLU:O	1:C:416:ARG:HG3	2.04	0.57
1:E:502:TYR:O	1:E:503:ALA:HB3	2.05	0.57
1:E:406:VAL:CA	1:E:409:LEU:HD13	2.30	0.56
1:A:176:ARG:CD	1:A:503:ALA:CA	2.41	0.56
1:E:434:VAL:HA	1:E:435:PRO:O	2.06	0.56
1:E:224:GLU:C	1:E:226:GLN:H	2.13	0.56
1:E:471:LEU:CD1	1:E:479:VAL:HG21	2.36	0.56
1:A:94:ASP:OD1	1:A:94:ASP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLU:O	1:A:337:ARG:HG3	2.05	0.56
1:C:287:MET:HE2	1:C:287:MET:CA	2.25	0.56
1:A:203:LYS:NZ	5:A:604:BGC:O6	2.38	0.56
1:C:123:GLY:N	1:C:128:ARG:O	2.22	0.56
1:C:280:LEU:HD23	1:C:280:LEU:N	2.11	0.56
1:A:147:THR:HG22	1:A:149:MET:H	1.70	0.56
1:A:352:VAL:O	1:A:352:VAL:HG23	2.03	0.56
1:C:176:ARG:NE	1:C:503:ALA:HB2	2.21	0.56
1:A:79:ARG:O	1:A:80:ALA:HB3	2.05	0.56
1:A:309:ALA:O	1:A:313:GLU:HG3	2.06	0.55
1:C:134:TYR:CD1	1:C:134:TYR:C	2.85	0.55
1:A:281:LEU:O	1:A:282:PRO:C	2.47	0.55
1:E:371:MET:HE1	1:E:386:LEU:HG	1.86	0.55
1:C:75:GLU:O	1:C:79:ARG:HG2	2.07	0.55
1:A:436:SER:C	1:A:439:SER:HA	2.32	0.55
1:E:283:ARG:H	1:E:283:ARG:CD	2.13	0.55
1:E:371:MET:HE1	1:E:386:LEU:CD2	2.37	0.55
1:C:258:ILE:HD13	1:C:449:ASP:HB3	1.89	0.55
1:A:119:ARG:NH2	1:A:162:PHE:O	2.39	0.55
1:A:380:LYS:NZ	1:A:380:LYS:HB3	2.22	0.55
1:E:433:ARG:HH21	1:E:433:ARG:CG	2.19	0.55
1:E:296:PHE:O	1:E:322:TYR:HB2	2.07	0.55
1:E:109:ASP:HB3	1:E:116:ARG:HG3	1.89	0.55
1:E:243:LEU:CD1	1:E:253:VAL:HG12	2.36	0.55
1:E:258:ILE:HD13	1:E:449:ASP:HB3	1.88	0.54
1:E:106:TYR:CG	1:E:230:MET:HE1	2.42	0.54
1:E:119:ARG:NH2	1:E:162:PHE:O	2.41	0.54
1:C:51:GLU:O	1:C:55:ARG:CG	2.46	0.54
1:A:134:TYR:C	1:A:134:TYR:CD1	2.85	0.54
1:E:134:TYR:CD1	1:E:134:TYR:C	2.86	0.54
1:C:236:VAL:O	1:C:237:ASN:O	2.25	0.54
1:C:437:ASP:CA	1:C:438:GLY:C	2.80	0.54
1:A:320:GLN:NE2	1:A:323:GLU:OE1	2.38	0.54
1:E:269:GLU:HG3	1:E:270:HIS:N	2.23	0.54
1:C:106:TYR:OH	1:C:166:GLU:HG3	2.08	0.54
1:E:104:LEU:HD22	1:E:105:PHE:N	2.23	0.54
1:E:40:GLU:O	1:E:42:ARG:N	2.40	0.54
1:E:490:ILE:HD12	1:E:494:LEU:HD11	1.90	0.54
1:C:442:GLN:O	1:C:478:SER:HB2	2.08	0.53
1:E:82:PRO:O	1:E:83:HIS:HB2	2.07	0.53
1:C:224:GLU:C	1:C:226:GLN:N	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLU:O	1:C:226:GLN:N	2.40	0.53
1:E:58:THR:HG22	1:E:302:PRO:HG3	1.91	0.53
1:C:118:ILE:HG22	1:C:119:ARG:N	2.23	0.53
1:A:119:ARG:HH22	1:A:165:THR:HG23	1.74	0.53
1:C:110:LEU:C	1:C:185:SER:HG	2.13	0.53
1:A:176:ARG:HD3	1:A:503:ALA:CB	2.33	0.53
1:E:169:ASP:OD1	1:E:169:ASP:N	2.39	0.53
1:A:247:ARG:O	1:A:247:ARG:HG3	2.07	0.53
1:A:397:LEU:O	1:A:401:TYR:HD1	1.92	0.53
1:C:40:GLU:C	1:C:42:ARG:N	2.63	0.52
1:E:432:ASP:OD1	1:E:432:ASP:N	2.31	0.52
1:A:160:GLU:HG3	1:A:161:SER:N	2.23	0.52
1:A:457:LYS:NZ	1:A:457:LYS:CB	2.72	0.52
1:E:101:GLU:HG3	1:E:494:LEU:CD2	2.40	0.52
1:C:453:TYR:CE1	1:C:460:ARG:HG3	2.45	0.52
1:A:106:TYR:CG	1:A:230:MET:HE1	2.45	0.52
1:A:176:ARG:CD	1:A:503:ALA:C	2.83	0.52
1:E:180:LEU:HD22	1:E:223:MET:CE	2.38	0.52
1:C:434:VAL:HG13	1:C:435:PRO:HD2	1.91	0.51
1:E:224:GLU:C	1:E:226:GLN:N	2.67	0.51
1:C:166:GLU:CD	1:C:178:ARG:NH1	2.54	0.51
1:A:39:GLU:CG	1:A:40:GLU:N	2.70	0.51
1:E:473:GLU:H	1:E:473:GLU:CD	2.17	0.51
1:C:163:VAL:O	1:C:166:GLU:HB2	2.11	0.51
1:C:312:PHE:CE2	1:A:141:PRO:HD3	2.46	0.51
1:C:437:ASP:H	1:C:438:GLY:HA2	1.70	0.51
1:A:433:ARG:O	1:A:433:ARG:HG3	2.11	0.51
1:E:261:THR:OG1	2:E:601:ADP:O3'	2.23	0.51
1:C:55:ARG:HD2	1:C:55:ARG:N	2.24	0.51
1:E:468:ALA:O	1:E:471:LEU:O	2.29	0.50
1:A:162:PHE:O	1:A:165:THR:HG22	2.10	0.50
1:E:220:SER:O	1:E:224:GLU:HG3	2.12	0.50
1:C:180:LEU:HD22	1:C:223:MET:CE	2.28	0.50
1:A:357:LEU:HB2	1:A:390:LEU:HD22	1.94	0.50
1:A:380:LYS:HB3	1:A:380:LYS:HZ2	1.75	0.50
1:C:58:THR:OG1	1:C:416:ARG:HD3	2.12	0.50
1:C:43:ARG:C	1:C:43:ARG:CD	2.85	0.50
1:C:102:HIS:HA	1:C:122:LEU:O	2.12	0.50
1:C:127:LYS:O	1:C:128:ARG:HB2	2.12	0.50
1:A:438:GLY:N	1:A:439:SER:CA	2.73	0.50
1:E:101:GLU:HB2	1:E:122:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ASP:CG	1:E:443:ARG:HH21	2.20	0.50
1:A:120:VAL:HG11	1:A:490:ILE:HD13	1.93	0.49
1:E:252:ASP:CB	1:E:445:VAL:HG23	2.43	0.49
1:C:49:ILE:O	1:C:53:GLU:HG2	2.12	0.49
1:E:49:ILE:HD11	1:E:402:ILE:HG23	1.94	0.49
1:C:79:ARG:O	1:C:80:ALA:HB3	2.11	0.49
1:A:378:ASP:O	1:A:400:ARG:NH2	2.45	0.49
1:A:471:LEU:HD13	1:A:476:ALA:HA	1.94	0.49
1:C:111:GLY:HA3	1:C:114:ASN:O	2.12	0.49
1:E:147:THR:HG22	1:E:149:MET:H	1.77	0.49
1:C:153:ASP:OD1	1:C:225:ARG:NH2	2.29	0.49
1:C:280:LEU:HG	1:C:280:LEU:O	2.13	0.49
1:C:390:LEU:HB2	1:C:392:VAL:HG22	1.94	0.49
1:A:134:TYR:CD1	1:A:135:GLU:N	2.81	0.49
1:E:224:GLU:O	1:E:226:GLN:N	2.46	0.49
1:A:408:ASP:O	1:A:412:GLU:HB2	2.13	0.49
1:A:501:GLN:N	1:A:502:TYR:CA	2.72	0.49
1:E:107:ALA:HB3	1:E:118:ILE:HB	1.94	0.49
1:C:442:GLN:CD	1:C:442:GLN:H	2.08	0.48
1:C:106:TYR:HB2	1:C:230:MET:HE1	1.94	0.48
1:C:261:THR:OG1	2:C:601:ADP:O3B	2.23	0.48
1:C:351:ASP:C	1:C:352:VAL:CG1	2.85	0.48
1:A:90:ILE:CG2	1:A:287:MET:HE2	2.39	0.48
1:C:107:ALA:HB2	1:C:493:ALA:HB2	1.96	0.48
1:C:283:ARG:CD	1:C:283:ARG:N	2.72	0.48
1:C:173:PRO:HD2	1:C:176:ARG:HD3	1.96	0.48
1:E:41:ARG:HD2	1:E:346:ALA:O	2.13	0.48
1:C:87:LYS:HB3	1:C:89:LEU:CD2	2.44	0.48
1:C:147:THR:HG22	1:C:149:MET:N	2.28	0.48
1:C:159:LEU:HD13	1:C:223:MET:HE3	1.95	0.48
1:C:443:ARG:NH2	1:C:445:VAL:HG21	2.27	0.48
1:E:462:CYS:O	1:E:466:THR:OG1	2.25	0.48
1:E:470:LEU:HA	1:E:470:LEU:HD23	1.74	0.48
1:E:454:GLU:OE1	1:E:455:HIS:CE1	2.66	0.48
1:E:450:GLY:O	1:E:454:GLU:HB2	2.13	0.48
1:C:114:ASN:ND2	1:C:136:GLU:OE1	2.47	0.47
1:C:122:LEU:CD1	1:C:494:LEU:HD23	2.44	0.47
1:A:162:PHE:O	1:A:165:THR:HG23	2.13	0.47
1:E:250:ASP:CG	1:E:443:ARG:NH2	2.72	0.47
1:A:65:GLY:O	1:A:300:ARG:NH1	2.47	0.47
1:E:364:ARG:HB3	1:E:366:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:TYR:HD1	1:A:135:GLU:N	2.12	0.47
1:E:106:TYR:HB2	1:E:230:MET:HE2	1.96	0.47
1:A:165:THR:O	1:A:165:THR:OG1	2.27	0.47
1:E:50:GLU:O	1:E:54:GLN:HG2	2.14	0.47
1:E:70:MET:O	1:E:74:MET:HG3	2.15	0.47
1:C:287:MET:CE	1:C:287:MET:CA	2.85	0.47
1:C:307:ASP:OD2	1:C:413:ARG:NH2	2.48	0.47
1:E:79:ARG:O	1:E:80:ALA:CB	2.59	0.47
1:A:106:TYR:CE1	1:A:163:VAL:HG12	2.50	0.47
1:A:434:VAL:CG2	1:A:474:GLU:OE2	2.59	0.46
1:E:116:ARG:HE	1:E:136:GLU:HG3	1.80	0.46
1:A:88:MET:HE3	1:A:289:ILE:HG21	1.97	0.46
1:A:110:LEU:HD23	1:A:184:PHE:CD1	2.51	0.46
1:C:482:LYS:HE2	1:C:482:LYS:HB3	1.61	0.46
1:E:40:GLU:C	1:E:42:ARG:N	2.74	0.46
1:E:433:ARG:NH2	1:E:433:ARG:CG	2.78	0.46
1:E:490:ILE:CD1	1:E:494:LEU:HG	2.46	0.46
1:C:267:TYR:HD1	1:C:429:LEU:HD21	1.80	0.46
1:C:269:GLU:CG	1:C:270:HIS:H	2.26	0.46
1:E:397:LEU:HD22	1:E:397:LEU:O	2.15	0.46
1:C:110:LEU:HD12	1:C:139:ILE:HD11	1.98	0.46
1:E:104:LEU:HD22	1:E:104:LEU:C	2.41	0.46
1:E:277:TRP:HA	1:E:277:TRP:CE3	2.51	0.46
1:A:86:LEU:HD22	1:A:293:TRP:HA	1.97	0.45
1:A:180:LEU:HD23	1:A:232:VAL:HG22	1.98	0.45
1:C:39:GLU:HB2	1:C:41:ARG:HG2	1.98	0.45
1:E:88:MET:HE3	1:E:289:ILE:HG21	1.99	0.45
1:E:147:THR:HG22	1:E:149:MET:N	2.32	0.45
1:A:105:PHE:CZ	1:A:497:ALA:HA	2.51	0.45
1:E:490:ILE:HD12	1:E:494:LEU:CD1	2.46	0.45
1:E:455:HIS:HB3	2:E:601:ADP:N6	2.31	0.45
1:A:120:VAL:CG1	1:A:132:GLN:HG3	2.33	0.45
1:A:445:VAL:HG22	1:A:480:VAL:HB	1.98	0.45
1:A:110:LEU:HD23	1:A:184:PHE:CE1	2.51	0.45
1:E:293:TRP:CD1	1:E:293:TRP:C	2.95	0.45
1:E:473:GLU:N	1:E:473:GLU:CD	2.72	0.45
1:C:58:THR:HG22	1:C:302:PRO:HG3	1.97	0.45
1:C:159:LEU:HD13	1:C:223:MET:CE	2.47	0.45
1:A:293:TRP:CD1	1:A:293:TRP:C	2.95	0.45
1:C:70:MET:O	1:C:74:MET:HG3	2.17	0.44
1:C:176:ARG:CB	1:C:503:ALA:HB1	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ASN:HB3	5:C:604:BGC:H5	1.99	0.44
1:A:440:GLN:HA	1:A:440:GLN:OE1	2.17	0.44
1:C:43:ARG:HD2	1:C:44:ARG:N	2.32	0.44
1:C:296:PHE:O	1:C:322:TYR:HB2	2.17	0.44
1:C:263:THR:HG22	1:C:323:GLU:HG3	1.99	0.44
1:C:301:LEU:HB3	1:C:325:MET:HE1	1.99	0.44
1:C:373:HIS:CD2	1:C:458:LYS:HG3	2.52	0.44
1:A:102:HIS:HD2	1:A:123:GLY:O	2.00	0.44
1:A:176:ARG:HD2	1:A:503:ALA:C	2.43	0.44
1:A:262:GLY:HA2	1:A:327:SER:HG	1.82	0.44
1:E:264:ASN:HA	1:E:293:TRP:CD1	2.52	0.44
1:A:92:TYR:H	1:A:287:MET:CE	2.31	0.44
1:A:328:GLY:O	1:A:365:THR:OG1	2.32	0.44
1:C:178:ARG:HB3	1:C:230:MET:HE2	2.00	0.43
1:C:373:HIS:NE2	1:C:457:LYS:HB3	2.33	0.43
1:A:40:GLU:O	1:A:41:ARG:C	2.60	0.43
1:E:371:MET:HE1	1:E:386:LEU:CG	2.48	0.43
1:C:160:GLU:OE2	1:C:164:LYS:HD2	2.18	0.43
1:A:264:ASN:ND2	5:A:604:BGC:O4	2.43	0.43
1:E:502:TYR:O	1:E:503:ALA:CB	2.66	0.43
1:E:110:LEU:O	1:E:185:SER:N	2.46	0.43
1:E:426:LEU:HD21	1:E:446:ILE:HD11	1.99	0.43
1:E:485:ASN:O	1:E:486:ASP:C	2.61	0.43
1:A:147:THR:HG22	1:A:149:MET:N	2.32	0.43
1:C:96:LEU:HD23	1:C:96:LEU:HA	1.87	0.43
1:A:457:LYS:O	1:A:458:LYS:C	2.58	0.43
1:E:283:ARG:N	1:E:283:ARG:CD	2.77	0.43
1:C:119:ARG:NH2	1:C:162:PHE:O	2.52	0.43
1:C:293:TRP:CD1	1:C:293:TRP:C	2.96	0.43
1:C:434:VAL:CG1	1:C:435:PRO:CD	2.85	0.43
1:A:76:ARG:HH21	1:A:85:PRO:HD3	1.83	0.43
1:A:397:LEU:HD11	1:A:401:TYR:HE1	1.83	0.43
1:A:436:SER:O	1:A:439:SER:HA	2.19	0.43
1:A:176:ARG:HH11	1:A:176:ARG:CG	2.31	0.42
1:E:270:HIS:C	1:E:272:ASN:H	2.26	0.42
1:C:201:TRP:C	1:C:202:THR:HG23	2.44	0.42
1:C:445:VAL:HG22	1:C:480:VAL:HB	2.02	0.42
1:E:252:ASP:HB3	1:E:445:VAL:HG23	2.00	0.42
1:C:267:TYR:CD1	1:C:429:LEU:HD21	2.53	0.42
1:A:127:LYS:HD3	1:A:127:LYS:HA	1.73	0.42
1:A:247:ARG:HA	1:A:250:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:THR:HG23	2:A:601:ADP:PB	2.60	0.42
1:C:223:MET:HG2	1:C:228:LEU:HD13	2.01	0.42
1:A:295:ASN:HA	1:A:320:GLN:HA	2.01	0.42
1:A:356:LYS:HD3	1:A:389:ILE:O	2.19	0.42
1:E:324:LYS:HA	1:E:330:TYR:CD1	2.53	0.42
1:E:174:GLU:H	1:E:174:GLU:HG3	1.58	0.42
1:E:86:LEU:HD21	1:E:296:PHE:HB2	2.02	0.42
1:A:457:LYS:NZ	1:A:457:LYS:HB2	2.34	0.42
1:C:40:GLU:C	1:C:42:ARG:H	2.27	0.42
1:C:51:GLU:O	1:C:51:GLU:HG2	2.19	0.42
1:C:207:ILE:HD13	1:C:207:ILE:HG21	1.85	0.42
1:C:264:ASN:HA	1:C:293:TRP:CD1	2.55	0.42
1:C:283:ARG:HD3	1:C:283:ARG:N	2.17	0.42
1:A:40:GLU:O	1:A:43:ARG:HG3	2.20	0.42
1:A:91:SER:O	1:A:92:TYR:HB2	2.18	0.42
1:E:247:ARG:HA	1:E:250:ASP:O	2.20	0.42
1:E:320:GLN:HE21	1:E:323:GLU:CD	2.28	0.42
1:C:358:GLU:OE2	1:A:356:LYS:HE3	2.20	0.41
1:E:110:LEU:HA	1:E:111:GLY:HA3	1.70	0.41
1:A:457:LYS:CB	1:A:457:LYS:HZ3	2.33	0.41
1:E:238:ASP:OD2	5:E:604:BGC:H6C1	2.20	0.41
1:E:434:VAL:CA	1:E:435:PRO:O	2.68	0.41
1:C:106:TYR:CD1	1:C:119:ARG:HB2	2.56	0.41
1:E:253:VAL:HA	1:E:445:VAL:HB	2.01	0.41
1:E:378:ASP:O	1:E:400:ARG:NH2	2.47	0.41
1:E:445:VAL:HG12	1:E:446:ILE:N	2.35	0.41
1:C:90:ILE:H	1:C:90:ILE:HG12	1.65	0.41
1:C:183:THR:HG21	1:C:488:SER:HB2	2.02	0.41
1:E:352:VAL:O	1:E:352:VAL:HG23	2.19	0.41
1:C:237:ASN:CG	1:C:238:ASP:N	2.72	0.41
1:E:270:HIS:C	1:E:272:ASN:N	2.78	0.41
1:A:159:LEU:CD1	1:A:223:MET:HE3	2.51	0.41
1:E:43:ARG:HG3	1:E:44:ARG:H	1.83	0.41
1:E:173:PRO:HB2	1:E:176:ARG:HG3	2.03	0.41
1:C:82:PRO:O	1:C:83:HIS:HB2	2.20	0.41
1:C:160:GLU:OE2	1:C:164:LYS:HE2	2.21	0.41
1:A:386:LEU:O	1:A:390:LEU:HB2	2.19	0.41
1:A:473:GLU:N	1:A:473:GLU:CD	2.78	0.41
1:E:267:TYR:OH	1:E:269:GLU:OE1	2.27	0.41
1:C:301:LEU:CD1	1:C:325:MET:HE1	2.47	0.41
1:A:159:LEU:O	1:A:160:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:GLN:HG3	1:E:192:SER:O	2.21	0.41
1:E:333:GLU:O	1:E:337:ARG:HG3	2.21	0.41
1:C:118:ILE:CG2	1:C:119:ARG:N	2.83	0.40
1:C:371:MET:HE3	1:C:389:ILE:HD12	2.03	0.40
1:C:484:ALA:O	1:C:485:ASN:C	2.61	0.40
1:A:296:PHE:O	1:A:322:TYR:HB2	2.20	0.40
1:A:436:SER:O	1:A:439:SER:CB	2.67	0.40
1:C:236:VAL:HG23	1:C:237:ASN:O	2.21	0.40
1:C:185:SER:O	5:C:604:BGC:O3	2.40	0.40
1:A:473:GLU:CD	1:A:473:GLU:H	2.29	0.40
1:E:58:THR:HB	1:E:63:LEU:HD21	2.03	0.40
1:E:386:LEU:HD22	1:E:390:LEU:HD11	2.02	0.40
1:A:282:PRO:O	1:A:284:SER:N	2.53	0.40
1:E:247:ARG:NH2	1:E:253:VAL:O	2.53	0.40
1:C:122:LEU:HD11	1:C:494:LEU:HD23	2.02	0.40
1:C:419:ALA:HB2	1:C:463:LEU:HD22	2.03	0.40
1:A:176:ARG:CG	1:A:176:ARG:NH1	2.84	0.40
1:A:337:ARG:HH11	1:A:337:ARG:HD3	1.72	0.40
1:E:243:LEU:HD12	1:E:253:VAL:HG12	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:GLU:OE1	1:A:283:ARG:NH1[5_685]	1.46	0.74
1:C:477:SER:O	1:A:281:LEU:CD1[5_685]	1.59	0.61
1:C:272:ASN:ND2	1:C:272:ASN:ND2[4_555]	1.87	0.33

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	463/465 (100%)	444 (96%)	17 (4%)	2 (0%)	30	65
1	C	463/465 (100%)	438 (95%)	18 (4%)	7 (2%)	8	35
1	E	463/465 (100%)	438 (95%)	23 (5%)	2 (0%)	30	65
All	All	1389/1395 (100%)	1320 (95%)	58 (4%)	11 (1%)	16	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	439	SER
1	E	435	PRO
1	A	435	PRO
1	E	41	ARG
1	C	225	ARG
1	C	237	ASN
1	C	486	ASP
1	C	41	ARG
1	C	185	SER
1	A	436	SER
1	C	279	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	377/377 (100%)	328 (87%)	49 (13%)	4	19
1	C	377/377 (100%)	324 (86%)	53 (14%)	3	16
1	E	377/377 (100%)	328 (87%)	49 (13%)	4	19
All	All	1131/1131 (100%)	980 (87%)	151 (13%)	4	18

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	40	GLU
1	C	42	ARG

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Mol	Chain	Res	Type
1	C	44	ARG
1	C	53	GLU
1	C	76	ARG
1	C	81	ASP
1	C	86	LEU
1	C	89	LEU
1	C	91	SER
1	C	104	LEU
1	C	117	VAL
1	C	127	LYS
1	C	135	GLU
1	C	136	GLU
1	C	149	MET
1	C	159	LEU
1	C	161	SER
1	C	163	VAL
1	C	164	LYS
1	C	169	ASP
1	C	171	HIS
1	C	172	LEU
1	C	173	PRO
1	C	185	SER
1	C	203	LYS
1	C	210	THR
1	C	221	ARG
1	C	223	MET
1	C	224	GLU
1	C	228	LEU
1	C	230	MET
1	C	235	LEU
1	C	238	ASP
1	C	251	ASN
1	C	272	ASN
1	C	278	THR
1	C	283	ARG
1	C	287	MET
1	C	293	TRP
1	C	297	LYS
1	C	352	VAL
1	C	363	LEU
1	C	385	LYS
1	C	387	LYS

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Mol	Chain	Res	Type
1	C	395	THR
1	C	400	ARG
1	C	404	LEU
1	C	413	ARG
1	C	433	ARG
1	C	440	GLN
1	C	442	GLN
1	C	457	LYS
1	C	482	LYS
1	A	40	GLU
1	A	41	ARG
1	A	42	ARG
1	A	49	ILE
1	A	50	GLU
1	A	51	GLU
1	A	58	THR
1	A	91	SER
1	A	94	ASP
1	A	104	LEU
1	A	113	THR
1	A	114	ASN
1	A	121	GLN
1	A	129	VAL
1	A	130	VAL
1	A	149	MET
1	A	159	LEU
1	A	160	GLU
1	A	165	THR
1	A	169	ASP
1	A	172	LEU
1	A	176	ARG
1	A	177	GLN
1	A	210	THR
1	A	228	LEU
1	A	229	ASP
1	A	230	MET
1	A	247	ARG
1	A	251	ASN
1	A	261	THR
1	A	280	LEU
1	A	281	LEU
1	A	293	TRP

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Mol	Chain	Res	Type
1	A	304	SER
1	A	313	GLU
1	A	320	GLN
1	A	351	ASP
1	A	380	LYS
1	A	398	GLU
1	A	412	GLU
1	A	436	SER
1	A	441	LYS
1	A	448	LEU
1	A	452	LEU
1	A	457	LYS
1	A	463	LEU
1	A	469	ASP
1	A	473	GLU
1	A	502	TYR
1	E	39	GLU
1	E	43	ARG
1	E	51	GLU
1	E	75	GLU
1	E	81	ASP
1	E	101	GLU
1	E	104	LEU
1	E	125	ARG
1	E	129	VAL
1	E	135	GLU
1	E	136	GLU
1	E	159	LEU
1	E	169	ASP
1	E	172	LEU
1	E	174	GLU
1	E	193	ILE
1	E	210	THR
1	E	219	LEU
1	E	221	ARG
1	E	228	LEU
1	E	230	MET
1	E	249	VAL
1	E	272	ASN
1	E	281	LEU
1	E	283	ARG
1	E	287	MET

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Mol	Chain	Res	Type
1	E	293	TRP
1	E	325	MET
1	E	375	THR
1	E	380	LYS
1	E	390	LEU
1	E	394	ASP
1	E	395	THR
1	E	397	LEU
1	E	404	LEU
1	E	409	LEU
1	E	427	LYS
1	E	429	LEU
1	E	433	ARG
1	E	439	SER
1	E	442	GLN
1	E	443	ARG
1	E	444	THR
1	E	452	LEU
1	E	454	GLU
1	E	458	LYS
1	E	482	LYS
1	E	490	ILE
1	E	502	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	C	114	ASN
1	C	226	GLN
1	A	102	HIS
1	A	142	HIS
1	A	177	GLN
1	A	226	GLN
1	A	320	GLN
1	A	381	HIS
1	A	485	ASN
1	A	501	GLN
1	E	83	HIS
1	E	320	GLN
1	E	381	HIS
1	E	455	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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$
2	ADP	C	601	4	28,29,29	2.16	12 (42%)	43,45,45	1.86	9 (20%)
5	BGC	C	604	-	12,12,12	1.22	1 (8%)	17,17,17	0.84	0
2	ADP	A	601	4	28,29,29	2.52	11 (39%)	43,45,45	2.38	13 (30%)
2	ADP	E	601	4	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
3	PO4	C	602	-	4,4,4	0.96	0	6,6,6	0.46	0
5	BGC	A	604	-	12,12,12	1.42	1 (8%)	17,17,17	2.35	8 (47%)
3	PO4	A	602	-	4,4,4	0.96	0	6,6,6	0.46	0
5	BGC	E	604	-	12,12,12	1.17	1 (8%)	17,17,17	0.87	0
3	PO4	E	602	-	4,4,4	0.95	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	601	4	-	3/16/32/32	0/3/3/3
5	BGC	C	604	-	-	2/2/22/22	0/1/1/1
2	ADP	A	601	4	-	3/16/32/32	0/3/3/3
2	ADP	E	601	4	-	1/16/32/32	0/3/3/3
5	BGC	A	604	-	-	2/2/22/22	0/1/1/1
5	BGC	E	604	-	-	2/2/22/22	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ADP	PA-O3A	-6.76	1.52	1.59
2	C	601	ADP	C5-N7	-4.78	1.30	1.39
2	E	601	ADP	C5-C4	4.74	1.47	1.39
2	A	601	ADP	C8-N9	-4.53	1.29	1.37
2	C	601	ADP	C4-N9	-4.01	1.29	1.37
2	A	601	ADP	C5-N7	-3.84	1.32	1.39
2	C	601	ADP	C8-N9	-3.60	1.31	1.37
2	A	601	ADP	C4-N9	-3.59	1.30	1.37
2	A	601	ADP	PB-O3B	-3.32	1.42	1.54
5	C	604	BGC	O5-C1	3.21	1.50	1.42
2	C	601	ADP	O4'-C4'	-3.09	1.38	1.45
2	C	601	ADP	PB-O2B	-3.09	1.43	1.54
2	A	601	ADP	PB-O2B	-3.07	1.43	1.54
5	E	604	BGC	O5-C1	2.98	1.50	1.42
5	A	604	BGC	O1-C1	-2.87	1.30	1.39
2	C	601	ADP	PB-O3B	-2.80	1.44	1.54
2	E	601	ADP	C5-C6	2.75	1.48	1.41
2	A	601	ADP	C2-N3	-2.64	1.29	1.33
2	C	601	ADP	PA-O2A	-2.61	1.43	1.55
2	A	601	ADP	PA-O2A	-2.58	1.43	1.55
2	A	601	ADP	O4'-C4'	-2.50	1.39	1.45
2	C	601	ADP	C2-N1	-2.35	1.29	1.33
2	E	601	ADP	C8-N7	2.34	1.36	1.31
2	A	601	ADP	C3'-C4'	-2.32	1.47	1.53
2	E	601	ADP	C5-N7	-2.28	1.34	1.39
2	C	601	ADP	C2-N3	-2.23	1.30	1.33
2	C	601	ADP	C3'-C4'	-2.19	1.47	1.53
2	A	601	ADP	C2'-C3'	-2.15	1.47	1.53
2	C	601	ADP	PA-O1A	-2.07	1.43	1.50
2	C	601	ADP	PA-O3A	-2.05	1.57	1.59

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	ADP	C5-C4-N3	-5.83	118.70	126.72
5	A	604	BGC	O5-C1-C2	-5.78	100.13	110.30
2	A	601	ADP	C5-C4-N3	-5.75	118.81	126.72
2	A	601	ADP	C2'-C1'-N9	-5.67	99.23	113.30
2	A	601	ADP	N3-C4-N9	5.35	136.27	127.17
2	C	601	ADP	C5-C4-N3	-5.27	119.46	126.72
2	C	601	ADP	N3-C4-N9	4.95	135.59	127.17
2	A	601	ADP	C4-N9-C8	4.64	110.61	105.74
2	E	601	ADP	N3-C4-N9	4.62	135.03	127.17
2	A	601	ADP	O3'-C3'-C2'	-4.35	97.86	111.82
2	A	601	ADP	C3'-C2'-C1'	3.78	108.61	101.46
5	A	604	BGC	C1-C2-C3	-3.77	102.66	110.36
2	A	601	ADP	C2-N3-C4	3.74	120.97	111.83
2	E	601	ADP	C2-N3-C4	3.70	120.88	111.83
2	C	601	ADP	C2-N3-C4	3.69	120.84	111.83
2	C	601	ADP	N3-C2-N1	-3.48	123.32	128.58
2	E	601	ADP	C4-C5-N7	-3.46	106.63	110.58
2	C	601	ADP	C4-N9-C8	3.39	109.30	105.74
2	A	601	ADP	C4-C5-N7	-3.38	106.72	110.58
2	E	601	ADP	N3-C2-N1	-3.23	123.70	128.58
2	A	601	ADP	N3-C2-N1	-3.16	123.81	128.58
2	A	601	ADP	O2'-C2'-C3'	-3.13	101.78	111.82
5	A	604	BGC	C4-C3-C2	3.07	116.22	110.83
2	A	601	ADP	N9-C8-N7	-3.03	109.64	113.94
2	A	601	ADP	C5-N7-C8	2.94	108.08	103.45
5	A	604	BGC	O4-C4-C3	-2.72	103.96	110.38
2	C	601	ADP	C5-C6-N6	-2.64	116.76	123.29
2	E	601	ADP	C4-N9-C8	2.60	108.47	105.74
2	E	601	ADP	C5-N7-C8	2.56	107.47	103.45
2	E	601	ADP	C3'-C2'-C1'	2.56	106.30	101.46
2	C	601	ADP	N6-C6-N1	2.54	124.04	118.38
2	C	601	ADP	O3B-PB-O2B	2.51	117.22	107.80
5	A	604	BGC	O2-C2-C1	2.41	114.82	109.25
5	A	604	BGC	O2-C2-C3	2.37	115.95	110.38
2	C	601	ADP	N9-C8-N7	-2.32	110.64	113.94
2	A	601	ADP	C6-C5-N7	2.25	136.44	132.09
5	A	604	BGC	C1-O5-C5	-2.14	109.50	113.65
5	A	604	BGC	O3-C3-C4	-2.11	105.41	110.38
2	E	601	ADP	C6-C5-N7	2.08	136.10	132.09

There are no chirality outliers.

All (13) torsion outliers are listed below:

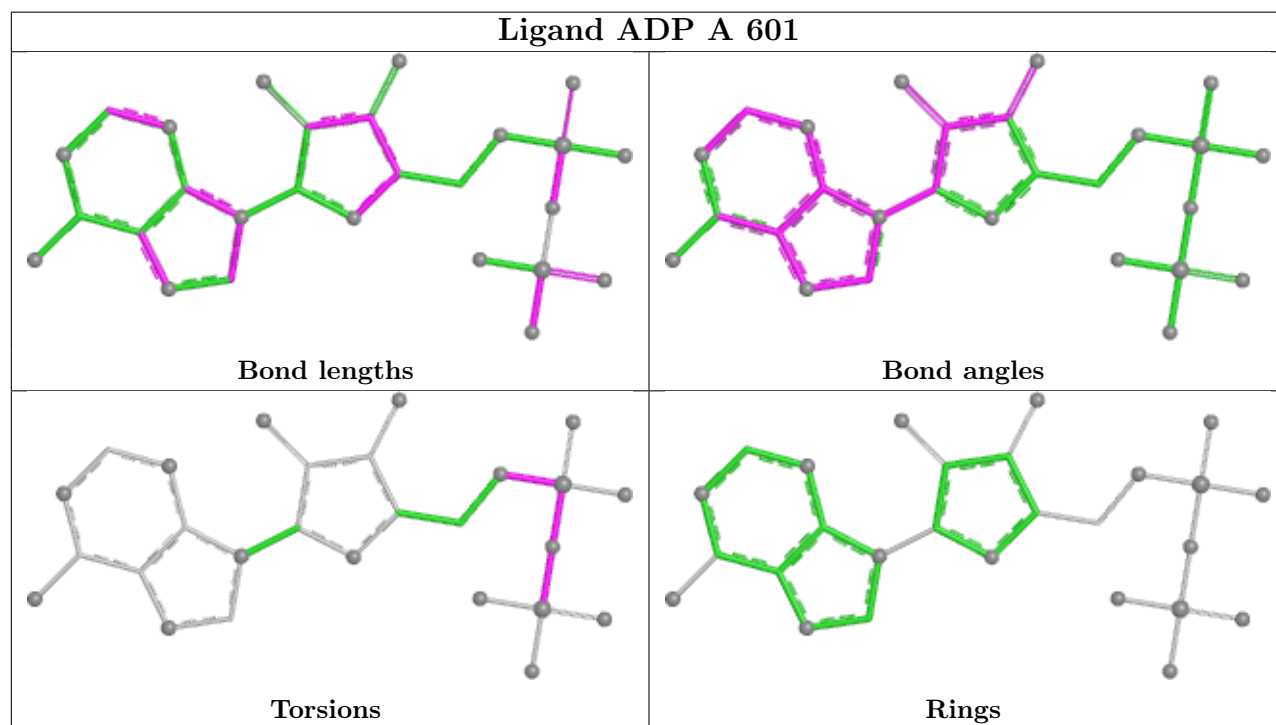
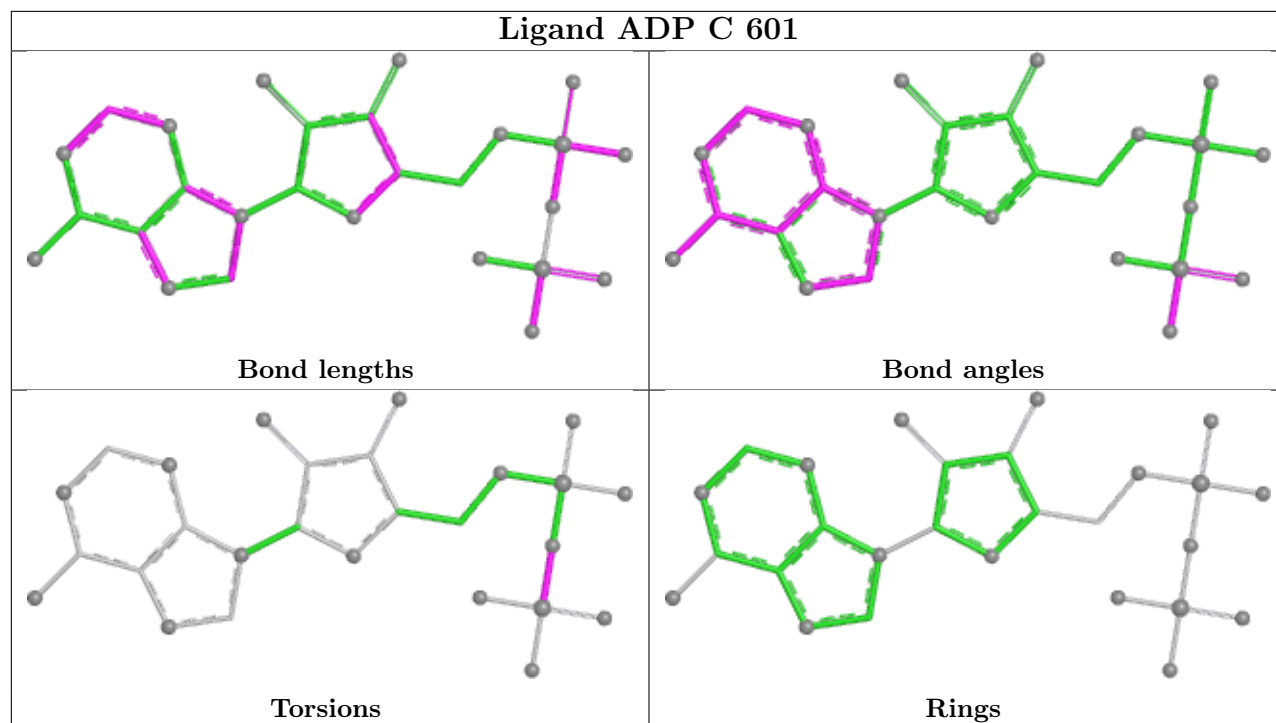
Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O1A
5	A	604	BGC	O5-C5-C6-O6
5	E	604	BGC	O5-C5-C6-O6
5	A	604	BGC	C4-C5-C6-O6
5	E	604	BGC	C4-C5-C6-O6
2	C	601	ADP	PA-O3A-PB-O1B
5	C	604	BGC	C4-C5-C6-O6
2	E	601	ADP	C3'-C4'-C5'-O5'
5	C	604	BGC	O5-C5-C6-O6
2	A	601	ADP	PB-O3A-PA-O2A
2	C	601	ADP	PA-O3A-PB-O2B
2	C	601	ADP	PA-O3A-PB-O3B
2	A	601	ADP	PA-O3A-PB-O3B

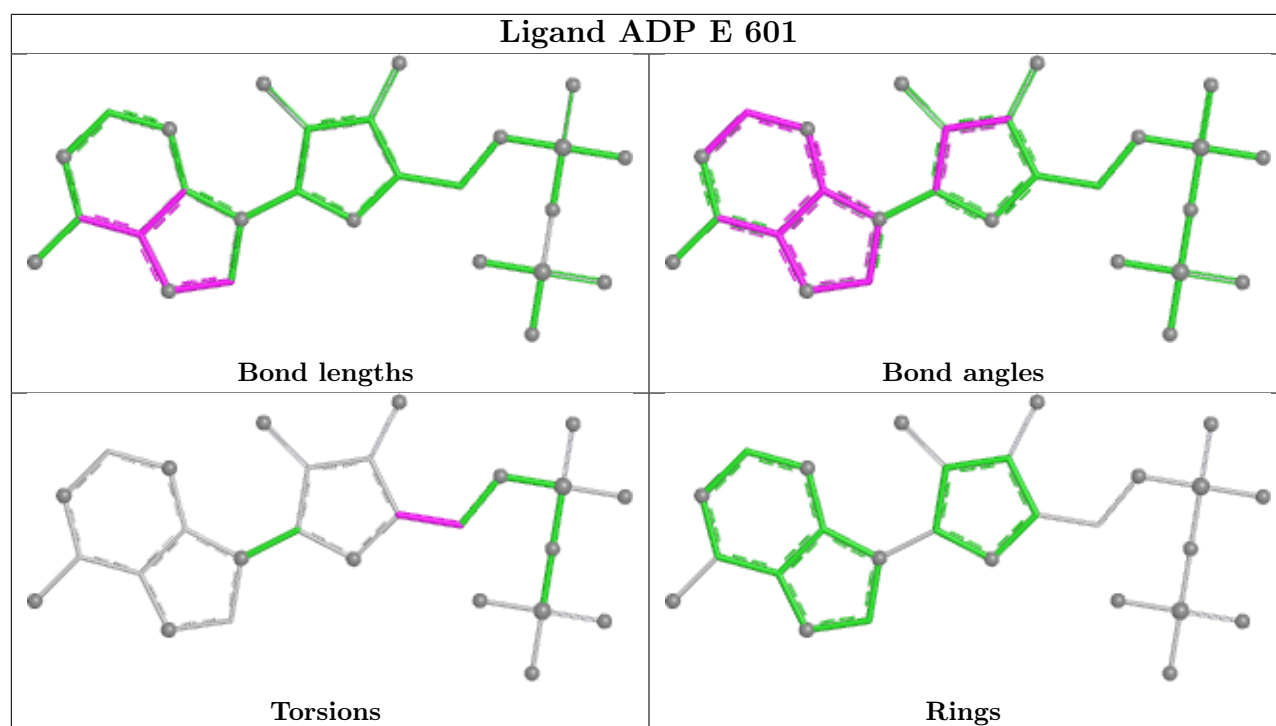
There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	ADP	1	0
5	C	604	BGC	5	0
2	A	601	ADP	3	0
2	E	601	ADP	3	0
5	A	604	BGC	4	0
5	E	604	BGC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/465 (100%)	-0.40	4 (0%) 81 61	12, 25, 52, 114	0
1	C	465/465 (100%)	-0.48	1 (0%) 91 83	12, 25, 52, 75	0
1	E	465/465 (100%)	-0.37	3 (0%) 85 69	17, 35, 58, 120	0
All	All	1395/1395 (100%)	-0.42	8 (0%) 85 69	12, 28, 55, 120	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	PRO	3.3
1	E	434	VAL	2.9
1	A	485	ASN	2.5
1	A	437	ASP	2.4
1	E	502	TYR	2.4
1	C	436	SER	2.3
1	E	438	GLY	2.2
1	A	438	GLY	2.1

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.

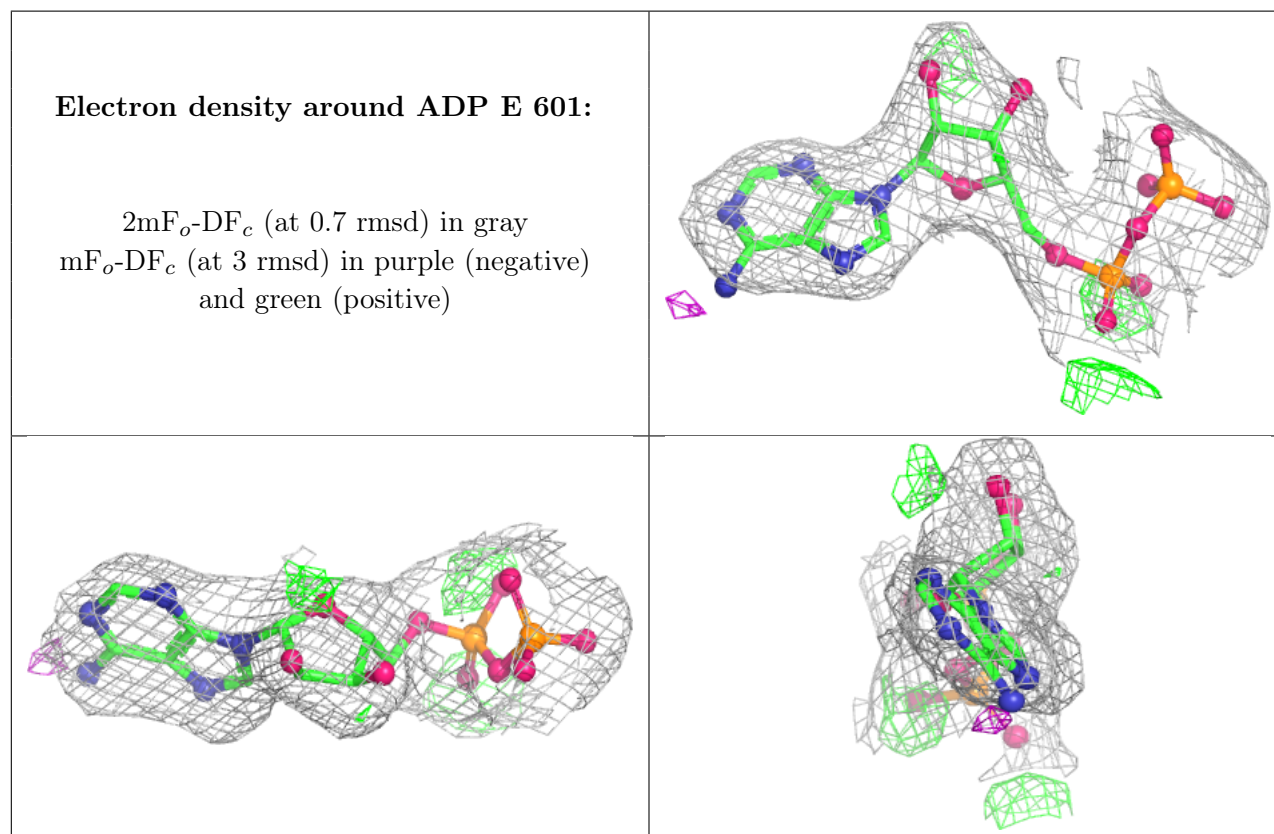
6.4 Ligands [i](#)

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.

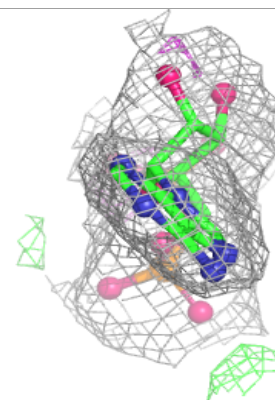
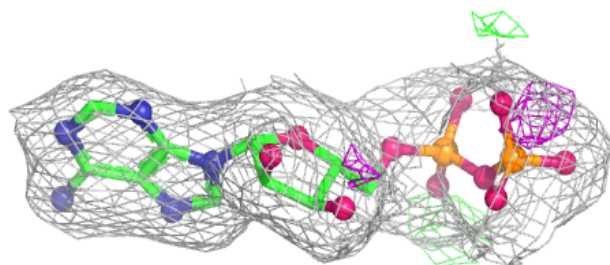
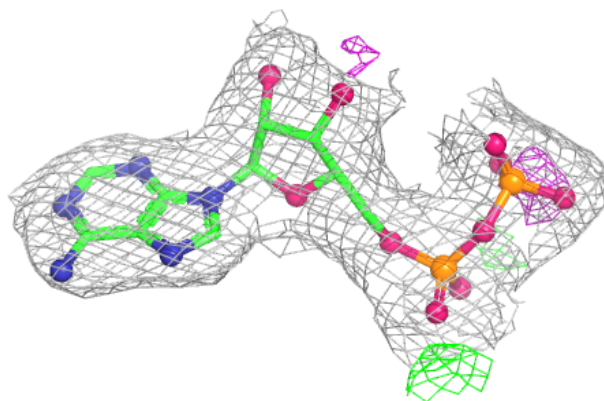
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	E	603	1/1	0.65	0.27	39,39,39,39	0
4	MG	C	603	1/1	0.79	0.30	43,43,43,43	0
4	MG	A	603	1/1	0.82	0.26	41,41,41,41	0
3	PO4	E	602	5/5	0.89	0.10	32,36,39,41	0
3	PO4	A	602	5/5	0.90	0.08	27,30,50,51	0
5	BGC	C	604	12/12	0.90	0.10	12,13,22,23	0
2	ADP	E	601	27/27	0.93	0.09	19,25,35,56	0
5	BGC	A	604	12/12	0.93	0.09	13,14,22,22	0
2	ADP	C	601	27/27	0.96	0.07	14,17,26,35	0
2	ADP	A	601	27/27	0.96	0.07	13,17,29,38	0
5	BGC	E	604	12/12	0.96	0.07	18,20,25,30	0
3	PO4	C	602	5/5	0.97	0.05	27,28,36,41	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.

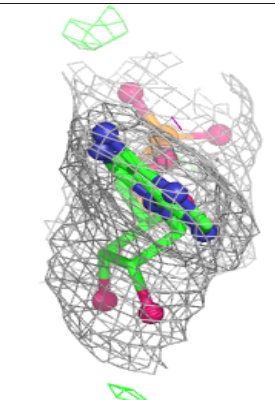
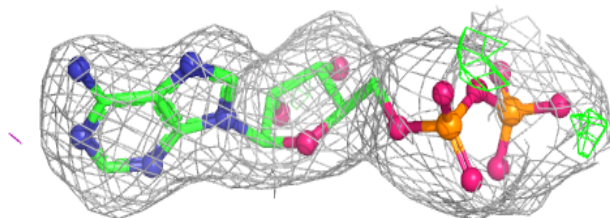
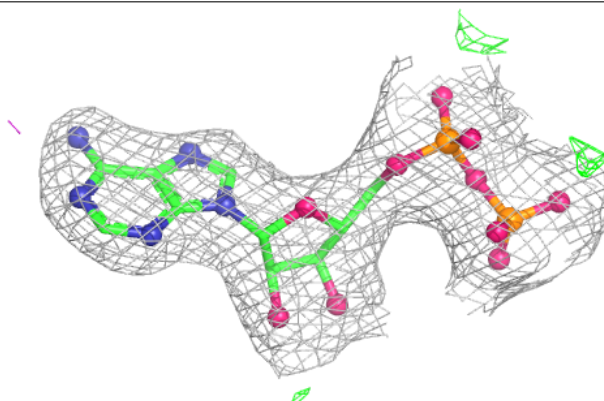


Electron density around ADP C 601:

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

**Electron density around ADP A 601:**

$2mF_o-DF_c$ (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.