



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:53 AM UTC

PDB ID : 1MV5 / pdb_00001mv5
Title : Crystal structure of LmrA ATP-binding domain
Authors : Yuan, Y.; Chen, H.; Patel, D.
Deposited on : 2002-09-24
Resolution : 3.10 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

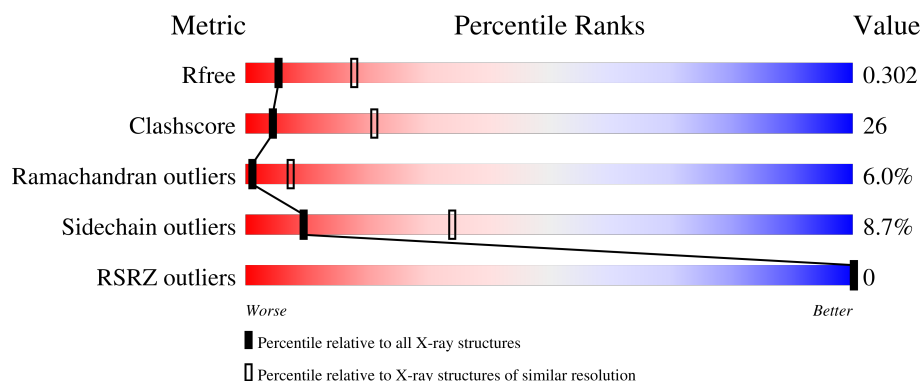
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

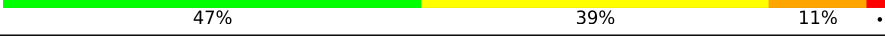
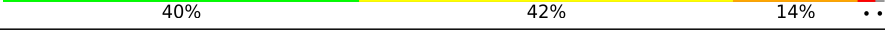
The reported resolution of this entry is 3.10 Å.

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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	243	
1	B	243	
1	C	243	
1	D	243	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7671 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.

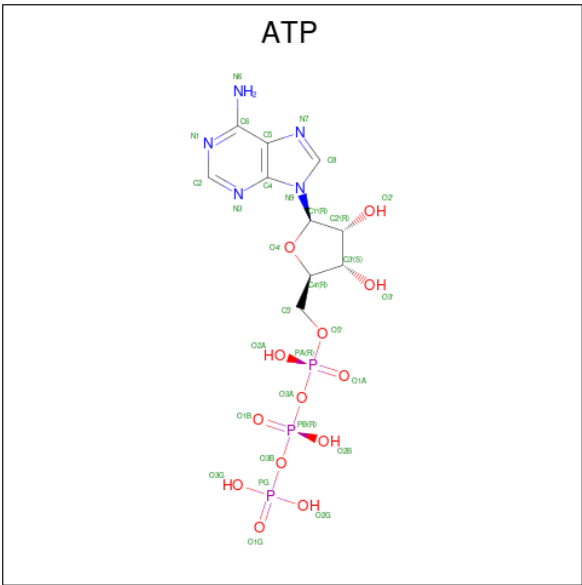
- Molecule 1 is a protein called Multidrug resistance ABC transporter ATP-binding and per-mease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1866	1174	321	365	6			
1	B	242	Total	C	N	O	S	0	0	0
			1877	1179	320	372	6			
1	C	242	Total	C	N	O	S	0	0	0
			1862	1172	321	363	6			
1	D	241	Total	C	N	O	S	0	0	0
			1870	1175	320	369	6			

There are 4 discrepancies between the modelled and reference sequences:

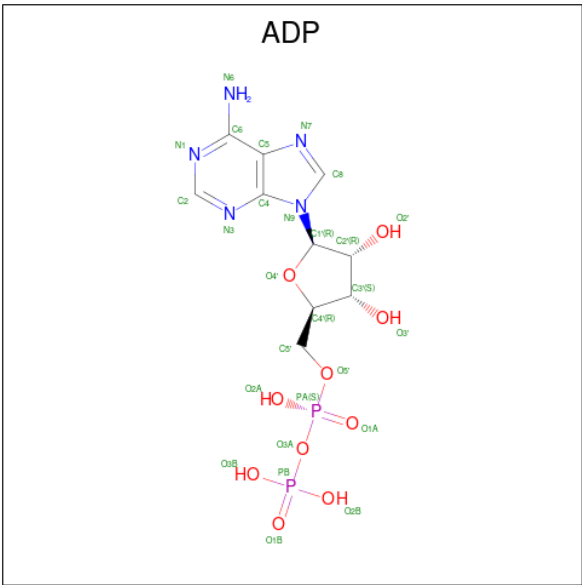
Chain	Residue	Modelled	Actual	Comment	Reference
A	342	MET	-	initiating methionine	UNP Q9CHL8
B	1342	MET	-	initiating methionine	UNP Q9CHL8
C	2342	MET	-	initiating methionine	UNP Q9CHL8
D	3342	MET	-	initiating methionine	UNP Q9CHL8

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- 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	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total 23	O 23	0	0
5	B	12	Total 12	O 12	0	0
5	C	24	Total 24	O 24	0	0
5	D	19	Total 19	O 19	0	0

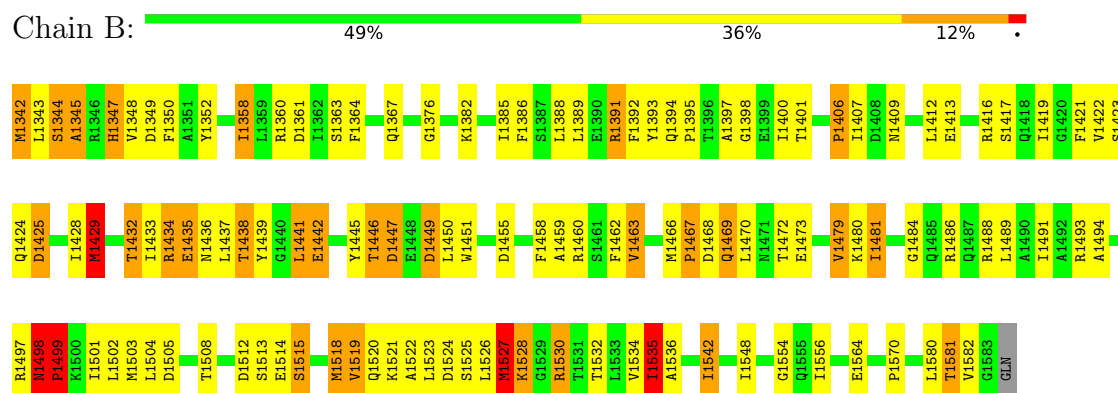
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

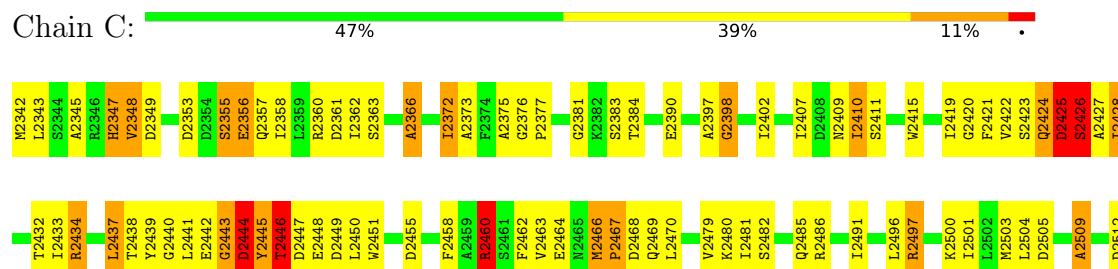
- Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein



- Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein



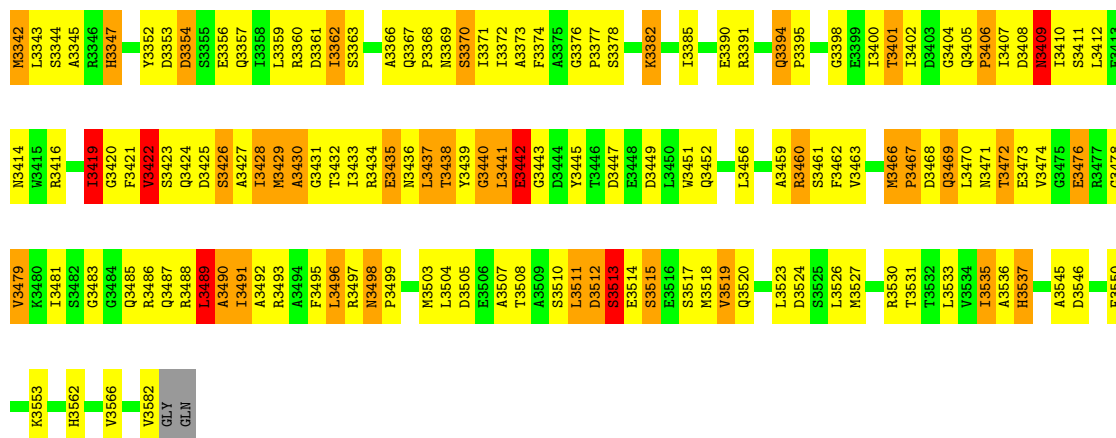
- Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein





- Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein

Chain D: 40% 42% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	141.87Å 141.87Å 120.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.10 40.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	84.8 (40.00-3.10) 95.5 (40.00-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.11Å)	Xtriage
Refinement program	X-PLOR 3.851, CNS	Depositor
R, R_{free}	0.251 , 0.283 0.270 , 0.302	Depositor DCC
R_{free} test set	1192 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.26	9/1897 (0.5%)	1.55	32/2566 (1.2%)
1	B	1.25	8/1908 (0.4%)	1.64	39/2580 (1.5%)
1	C	1.19	8/1893 (0.4%)	1.57	35/2561 (1.4%)
1	D	1.28	9/1901 (0.5%)	1.62	43/2570 (1.7%)
All	All	1.25	34/7599 (0.4%)	1.59	149/10277 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3342	MET	SD-CE	-13.11	1.46	1.79
1	B	1342	MET	SD-CE	13.08	2.12	1.79
1	A	518	MET	SD-CE	12.01	2.09	1.79
1	A	429	MET	SD-CE	10.39	2.05	1.79
1	D	3466	MET	SD-CE	10.05	2.04	1.79
1	A	503	MET	SD-CE	-9.25	1.56	1.79
1	C	2518	MET	SD-CE	8.00	1.99	1.79
1	A	444	ASP	CB-CG	7.13	1.69	1.52
1	D	3428	ILE	CA-CB	6.97	1.62	1.54
1	B	1527	MET	SD-CE	6.91	1.96	1.79
1	B	1519	VAL	CA-CB	6.71	1.61	1.54
1	C	2366	ALA	CA-CB	-6.00	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	ASP	CA-C	-5.88	1.45	1.52
1	D	3479	VAL	CA-CB	5.74	1.62	1.54
1	D	3474	VAL	CA-CB	5.66	1.62	1.54
1	D	3490	ALA	CA-CB	-5.63	1.44	1.53
1	C	2445	TYR	CA-C	5.59	1.61	1.52
1	B	1345	ALA	CA-CB	-5.56	1.45	1.52
1	A	463	VAL	CA-CB	5.54	1.60	1.54
1	B	1429	MET	SD-CE	-5.53	1.65	1.79
1	B	1479	VAL	CA-CB	5.51	1.61	1.54
1	C	2582	VAL	CA-CB	5.50	1.61	1.54
1	D	3429	MET	CG-SD	5.46	1.94	1.80
1	A	373	ALA	CA-CB	-5.40	1.44	1.53
1	C	2342	MET	SD-CE	5.34	1.93	1.79
1	C	2445	TYR	CA-CB	5.30	1.60	1.54
1	C	2533	LEU	C-O	-5.30	1.17	1.23
1	D	3409	ASN	CA-C	-5.22	1.45	1.52
1	A	533	LEU	C-O	-5.22	1.18	1.24
1	B	1518	MET	SD-CE	5.19	1.92	1.79
1	A	582	VAL	CA-CB	5.13	1.61	1.54
1	D	3373	ALA	CA-CB	-5.10	1.46	1.53
1	C	2373	ALA	CA-CB	-5.09	1.44	1.53
1	B	1556	ILE	CA-CB	5.05	1.60	1.54

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2445	TYR	CB-CA-C	15.72	125.39	109.83
1	A	438	THR	N-CA-C	14.74	129.03	110.61
1	B	1468	ASP	N-CA-C	-13.62	94.70	112.41
1	B	1358	ILE	N-CA-C	12.58	122.50	110.42
1	C	2509	ALA	N-CA-C	11.59	126.92	113.01
1	B	1528	LYS	N-CA-C	10.30	124.94	112.38
1	B	1417	SER	N-CA-C	9.74	121.98	111.36
1	D	3422	VAL	N-CA-C	9.73	122.37	108.17
1	C	2348	VAL	N-CA-C	9.67	121.38	109.30
1	C	2426	SER	N-CA-C	-9.66	90.22	110.80
1	A	466	MET	CA-C-N	9.65	131.91	119.84
1	A	466	MET	C-N-CA	9.65	131.91	119.84
1	B	1508	THR	N-CA-C	-9.48	102.32	112.93
1	A	528	LYS	N-CA-C	9.47	122.48	111.11
1	A	415	TRP	N-CA-C	-9.39	101.83	113.38
1	B	1505	ASP	N-CA-C	-9.17	91.65	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1467	PRO	N-CA-C	9.12	131.26	112.47
1	B	1413	GLU	N-CA-C	8.92	122.30	110.88
1	B	1530	ARG	N-CA-C	8.77	123.23	109.81
1	B	1535	ILE	N-CA-C	-8.75	93.21	106.42
1	A	580	LEU	N-CA-C	8.72	121.66	111.02
1	D	3512	ASP	N-CA-C	-8.63	92.88	108.58
1	D	3370	SER	N-CA-C	8.60	119.29	108.45
1	C	2425	ASP	N-CA-C	8.23	128.34	110.80
1	B	1445	TYR	N-CA-C	8.20	122.35	109.81
1	B	1581	THR	N-CA-C	8.18	121.47	110.35
1	A	399	GLU	N-CA-C	8.17	121.32	110.53
1	C	2347	HIS	N-CA-C	8.16	122.76	111.74
1	A	414	ASN	N-CA-C	-7.93	101.08	111.71
1	A	445	TYR	N-CA-C	-7.93	101.80	114.09
1	C	2500	LYS	N-CA-C	-7.92	103.23	113.12
1	C	2434	ARG	N-CA-C	-7.91	103.76	113.41
1	C	2443	GLY	N-CA-C	7.90	123.43	112.37
1	A	579	GLN	N-CA-C	7.86	119.75	111.03
1	B	1536	ALA	N-CA-C	7.64	120.82	109.59
1	A	408	ASP	N-CA-C	7.47	120.58	109.59
1	D	3535	ILE	N-CA-C	-7.43	96.05	106.53
1	C	2537	HIS	N-CA-C	-7.43	105.39	114.75
1	D	3378	SER	N-CA-C	7.29	120.15	111.33
1	C	2425	ASP	CA-C-N	7.19	135.27	121.54
1	C	2425	ASP	C-N-CA	7.19	135.27	121.54
1	B	1462	PHE	N-CA-C	-7.16	103.47	111.28
1	D	3545	ALA	N-CA-C	-7.13	101.11	110.53
1	B	1385	ILE	N-CA-C	-7.08	103.88	110.53
1	B	1518	MET	CB-CG-SD	-7.07	91.51	112.70
1	C	2569	HIS	CA-C-N	7.03	126.85	119.05
1	C	2569	HIS	C-N-CA	7.03	126.85	119.05
1	D	3491	ILE	N-CA-C	-6.94	102.14	111.44
1	A	410	ILE	CB-CA-C	6.85	122.53	111.29
1	C	2357	GLN	N-CA-C	-6.82	98.08	109.07
1	A	445	TYR	CB-CA-C	6.77	120.70	109.80
1	B	1401	THR	N-CA-C	6.75	119.51	108.52
1	D	3394	GLN	CA-C-N	6.74	128.26	119.84
1	D	3394	GLN	C-N-CA	6.74	128.26	119.84
1	D	3460	ARG	N-CA-C	6.70	118.24	111.07
1	C	2534	VAL	CB-CA-C	-6.62	100.75	110.81
1	D	3498	ASN	CA-C-N	6.58	126.54	120.03
1	D	3498	ASN	C-N-CA	6.58	126.54	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	GLY	N-CA-C	-6.57	100.33	110.77
1	D	3478	GLY	N-CA-C	6.56	120.97	112.18
1	D	3420	GLY	N-CA-C	-6.54	98.77	111.12
1	D	3472	THR	N-CA-C	6.52	120.91	109.96
1	A	551	ILE	N-CA-C	6.40	116.84	107.37
1	C	2535	ILE	N-CA-C	-6.38	97.38	107.15
1	D	3466	MET	CA-C-N	6.38	127.81	119.84
1	D	3466	MET	C-N-CA	6.38	127.81	119.84
1	B	1389	LEU	N-CA-C	-6.37	104.21	112.23
1	D	3519	VAL	N-CA-C	-6.35	104.30	110.72
1	D	3441	LEU	CA-C-N	-6.33	109.44	121.54
1	D	3441	LEU	C-N-CA	-6.33	109.44	121.54
1	B	1499	PRO	N-CA-C	6.32	125.49	112.47
1	D	3461	SER	N-CA-C	6.18	118.99	111.82
1	A	348	VAL	N-CA-C	6.17	117.04	108.89
1	C	2362	ILE	N-CA-C	6.15	117.64	108.54
1	C	2522	ALA	N-CA-C	-6.07	105.37	112.89
1	C	2466	MET	CA-C-N	6.06	127.42	119.84
1	C	2466	MET	C-N-CA	6.06	127.42	119.84
1	D	3515	SER	N-CA-C	-6.05	104.59	111.07
1	A	429	MET	N-CA-C	-6.03	98.59	108.41
1	B	1564	GLU	N-CA-C	-5.99	104.67	111.14
1	D	3435	GLU	N-CA-C	5.98	118.57	111.33
1	D	3442	GLU	CA-C-N	5.95	126.43	119.94
1	D	3442	GLU	C-N-CA	5.95	126.43	119.94
1	C	2512	ASP	N-CA-C	5.92	119.33	111.75
1	A	536	ALA	N-CA-C	5.92	119.04	110.28
1	B	1455	ASP	N-CA-C	-5.92	104.41	111.69
1	C	2424	GLN	N-CA-C	5.89	119.54	110.42
1	C	2444	ASP	N-CA-C	5.88	123.32	110.80
1	D	3537	HIS	N-CA-C	-5.87	104.79	112.41
1	B	1520	GLN	N-CA-C	5.85	120.11	113.15
1	A	414	ASN	CA-C-N	5.84	132.36	122.26
1	A	414	ASN	C-N-CA	5.84	132.36	122.26
1	C	2497	ARG	N-CA-C	-5.83	105.42	112.54
1	B	1512	ASP	N-CA-C	5.78	118.84	110.28
1	D	3489	LEU	N-CA-C	-5.78	106.08	113.01
1	B	1432	THR	N-CA-C	-5.76	100.55	109.24
1	D	3419	ILE	N-CA-C	5.75	115.94	108.35
1	A	463	VAL	N-CA-C	-5.74	107.39	112.90
1	D	3430	ALA	N-CA-C	-5.74	106.26	113.20
1	C	2428	ILE	CB-CA-C	-5.69	103.20	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3352	TYR	CA-CB-CG	5.69	124.14	113.90
1	B	1350	PHE	N-CA-C	5.66	117.88	108.99
1	A	475	GLY	CA-C-N	5.65	132.34	121.54
1	A	475	GLY	C-N-CA	5.65	132.34	121.54
1	B	1447	ASP	N-CA-C	-5.64	105.13	111.28
1	A	474	VAL	N-CA-C	5.64	116.70	108.53
1	D	3510	SER	N-CA-C	-5.61	99.65	108.63
1	B	1449	ASP	N-CA-C	-5.60	104.81	111.69
1	A	530	ARG	N-CA-C	5.58	122.68	110.80
1	D	3401	THR	N-CA-C	5.58	119.01	110.20
1	B	1498	ASN	N-CA-C	5.54	122.06	109.81
1	B	1554	GLY	N-CA-C	5.52	122.39	115.21
1	C	2358	ILE	N-CA-C	5.52	116.17	110.82
1	B	1582	VAL	N-CA-C	5.51	115.88	108.17
1	D	3411	SER	N-CA-C	-5.49	104.69	111.33
1	C	2572	TYR	N-CA-C	-5.46	105.41	111.36
1	B	1376	GLY	CA-C-N	5.44	125.37	119.76
1	B	1376	GLY	C-N-CA	5.44	125.37	119.76
1	B	1542	ILE	N-CA-CB	-5.41	104.50	110.51
1	D	3391	ARG	N-CA-C	5.41	119.18	112.47
1	C	2576	VAL	N-CA-C	5.39	117.83	111.09
1	A	519	VAL	N-CA-C	-5.39	104.22	111.44
1	D	3416	ARG	CA-C-N	5.35	127.99	120.28
1	D	3416	ARG	C-N-CA	5.35	127.99	120.28
1	C	2446	THR	N-CA-C	5.35	122.19	110.80
1	D	3496	LEU	N-CA-C	5.33	116.78	110.97
1	C	2514	GLU	N-CA-C	-5.33	107.14	113.97
1	A	347	HIS	N-CA-C	5.33	118.98	111.52
1	B	1513	SER	N-CA-C	5.32	122.12	110.80
1	C	2525	SER	N-CA-C	-5.30	106.65	113.23
1	B	1395	PRO	N-CA-C	-5.30	102.26	112.01
1	A	428	ILE	N-CA-C	-5.29	100.85	108.42
1	A	477	ARG	CB-CA-C	5.28	118.93	111.86
1	B	1423	SER	N-CA-C	-5.25	102.83	110.24
1	B	1425	ASP	N-CA-C	5.24	121.95	110.80
1	B	1435	GLU	N-CA-C	5.21	117.71	111.71
1	D	3536	ALA	N-CA-C	5.19	118.02	109.76
1	D	3553	LYS	N-CA-C	5.17	118.46	111.17
1	C	2445	TYR	N-CA-C	-5.16	105.66	113.51
1	D	3422	VAL	CA-C-O	5.16	126.05	120.43
1	A	391	ARG	N-CA-C	5.15	119.52	113.23
1	C	2581	THR	N-CA-C	5.11	116.66	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3456	LEU	N-CA-C	-5.08	107.25	113.50
1	A	415	TRP	N-CA-CB	-5.05	103.01	110.53
1	A	419	ILE	CB-CA-C	-5.03	104.34	111.38
1	C	2533	LEU	CA-CB-CG	5.03	133.90	116.30
1	D	3385	ILE	N-CA-C	-5.03	105.64	110.72
1	B	1441	LEU	N-CA-C	5.01	119.47	112.90
1	D	3505	ASP	N-CA-C	-5.00	99.67	107.93

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2572	TYR	Sidechain
1	D	3422	VAL	Mainchain

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	1866	0	1823	81	0
1	B	1877	0	1846	76	0
1	C	1862	0	1819	111	0
1	D	1870	0	1840	139	0
2	A	31	0	12	2	0
2	C	31	0	12	3	0
3	B	27	0	12	2	0
3	D	27	0	12	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	23	0	0	1	0
5	B	12	0	0	1	0
5	C	24	0	0	5	0
5	D	19	0	0	1	0
All	All	7671	0	7376	394	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 26.

All (394) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3466:MET:SD	1:D:3466:MET:CE	2.04	1.45
1:A:429:MET:SD	1:A:429:MET:CE	2.05	1.43
1:A:518:MET:CE	1:A:518:MET:SD	2.09	1.40
1:B:1342:MET:SD	1:B:1342:MET:CE	2.12	1.38
1:C:2539:LEU:HD11	5:C:4069:HOH:O	1.34	1.21
1:C:2438:THR:O	1:C:2441:LEU:HG	1.45	1.16
1:D:3342:MET:HE3	1:D:3367:GLN:HG2	1.30	1.13
1:D:3353:ASP:O	1:D:3354:ASP:CB	1.98	1.09
1:C:2518:MET:HA	1:C:2521:LYS:HE2	1.35	1.08
1:D:3353:ASP:O	1:D:3354:ASP:HB3	1.51	1.07
1:C:2446:THR:O	1:C:2449:ASP:OD1	1.69	1.07
1:D:3441:LEU:O	1:D:3497:ARG:NH2	1.95	0.99
1:D:3422:VAL:HG21	1:D:3490:ALA:HB1	1.45	0.98
1:B:1491:ILE:HG21	1:B:1522:ALA:HB1	1.46	0.96
1:C:2440:GLY:O	1:C:2441:LEU:HD23	1.68	0.93
1:C:2518:MET:CA	1:C:2521:LYS:HE2	2.00	0.92
1:A:439:TYR:H	1:A:493:ARG:HH12	1.17	0.90
1:D:3370:SER:HB2	1:D:3546:ASP:OD2	1.70	0.90
1:A:427:ALA:HB3	1:A:486:ARG:NH1	1.89	0.88
3:B:1600:ADP:H2'	1:C:2353:ASP:OD2	1.75	0.86
1:C:2563:ASN:OD1	1:C:2564:GLU:N	2.08	0.86
1:D:3342:MET:HE3	1:D:3367:GLN:CG	2.05	0.85
1:D:3441:LEU:CD1	1:D:3496:LEU:HD12	2.08	0.83
1:D:3342:MET:CE	1:D:3367:GLN:HG2	2.08	0.82
1:A:427:ALA:HB3	1:A:486:ARG:CZ	2.10	0.82
1:D:3422:VAL:CG2	1:D:3490:ALA:HB1	2.10	0.81
1:C:2518:MET:HA	1:C:2521:LYS:CE	2.11	0.80
1:D:3515:SER:O	1:D:3519:VAL:CG2	2.28	0.80
1:D:3515:SER:O	1:D:3519:VAL:HG23	1.80	0.80
1:C:2460:ARG:NH2	1:D:3428:ILE:HA	1.97	0.80
1:B:1481:ILE:HB	1:B:1486:ARG:HE	1.45	0.80
1:D:3343:LEU:HB3	1:D:3366:ALA:HB3	1.63	0.79
1:A:438:THR:HG22	1:A:438:THR:O	1.82	0.79
1:D:3441:LEU:CD1	1:D:3496:LEU:CD1	2.61	0.79
1:C:2349:ASP:HB2	1:C:2397:ALA:HB3	1.65	0.78
1:B:1526:LEU:HD22	1:B:1530:ARG:HH22	1.47	0.77
1:C:2518:MET:CB	1:C:2521:LYS:HE2	2.14	0.77
1:D:3431:GLY:O	1:D:3473:GLU:HG2	1.85	0.77
1:D:3422:VAL:HG11	1:D:3490:ALA:CB	2.14	0.77
1:D:3353:ASP:O	1:D:3354:ASP:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1434:ARG:HB2	1:B:1470:LEU:O	1.86	0.75
1:A:424:GLN:CG	1:A:486:ARG:HH21	1.99	0.75
1:C:2449:ASP:OD1	1:C:2450:LEU:N	2.19	0.75
1:C:2460:ARG:HH21	1:D:3428:ILE:HA	1.50	0.75
1:A:390:GLU:HG3	1:A:503:MET:HE1	1.68	0.75
1:A:506:GLU:HG3	1:A:537:HIS:HB2	1.68	0.74
1:B:1519:VAL:O	1:B:1523:LEU:HB2	1.87	0.74
1:B:1344:SER:OG	5:B:4063:HOH:O	1.97	0.74
1:C:2360:ARG:NH2	1:C:2553:LYS:O	2.22	0.73
1:C:2455:ASP:O	1:D:3439:TYR:OH	2.06	0.73
1:A:424:GLN:HG2	1:A:486:ARG:HH21	1.54	0.73
1:D:3515:SER:O	1:D:3519:VAL:CB	2.36	0.73
1:D:3441:LEU:HD11	1:D:3496:LEU:HD12	1.71	0.72
1:D:3515:SER:O	1:D:3519:VAL:HB	1.88	0.72
1:B:1421:PHE:CD1	1:B:1499:PRO:HG2	2.24	0.72
1:D:3442:GLU:H	1:D:3445:TYR:HE1	1.36	0.71
1:C:2518:MET:HA	1:C:2521:LYS:HG2	1.73	0.71
1:D:3491:ILE:HG23	1:D:3526:LEU:HD22	1.71	0.71
1:B:1400:ILE:HB	1:B:1407:ILE:HD12	1.72	0.71
1:A:526:LEU:O	1:A:530:ARG:HD3	1.90	0.70
1:B:1484:GLY:HA2	1:B:1518:MET:SD	2.32	0.69
1:B:1491:ILE:O	1:B:1494:ALA:HB3	1.93	0.69
1:C:2463:VAL:HA	1:C:2466:MET:HE2	1.73	0.69
1:D:3442:GLU:HB2	1:D:3445:TYR:OH	1.92	0.69
1:D:3422:VAL:CB	1:D:3490:ALA:HB1	2.24	0.67
1:B:1386:PHE:HE1	1:B:1504:LEU:O	1.77	0.67
1:B:1437:LEU:HD13	1:B:1489:LEU:HD22	1.76	0.67
1:C:2557:THR:HG22	5:C:4034:HOH:O	1.94	0.67
1:A:488:ARG:NH2	1:A:518:MET:HB2	2.10	0.67
1:D:3429:MET:HG3	1:D:3429:MET:O	1.94	0.66
1:D:3441:LEU:C	1:D:3497:ARG:HH21	2.02	0.66
1:C:2518:MET:HG2	1:C:2521:LYS:NZ	2.11	0.66
1:D:3421:PHE:HZ	1:D:3424:GLN:NE2	1.94	0.65
1:A:465:ASN:ND2	1:B:1422:VAL:HB	2.11	0.65
1:C:2415:TRP:CE2	1:C:2419:ILE:HD11	2.32	0.65
1:D:3437:LEU:HD21	1:D:3489:LEU:HD23	1.78	0.65
1:D:3462:PHE:CZ	1:D:3488:ARG:NH1	2.64	0.65
1:B:1466:MET:HB3	1:B:1472:THR:HG21	1.79	0.64
1:C:2424:GLN:HG3	1:C:2425:ASP:H	1.62	0.64
1:A:446:THR:HG22	1:A:448:GLU:H	1.61	0.64
1:A:479:VAL:HG12	1:A:480:LYS:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1347:HIS:O	1:B:1398:GLY:HA3	1.97	0.64
1:D:3511:LEU:O	1:D:3513:SER:N	2.31	0.64
1:C:2433:ILE:CD1	1:C:2466:MET:HE1	2.28	0.64
1:C:2557:THR:CG2	5:C:4034:HOH:O	2.46	0.63
1:D:3462:PHE:HZ	1:D:3488:ARG:HH12	1.46	0.63
1:B:1493:ARG:HH21	1:B:1497:ARG:NH2	1.97	0.63
1:D:3390:GLU:HG2	1:D:3503:MET:HE1	1.81	0.63
1:D:3511:LEU:C	1:D:3513:SER:N	2.57	0.62
1:D:3422:VAL:HG11	1:D:3490:ALA:HB2	1.81	0.62
1:D:3441:LEU:HD13	1:D:3496:LEU:HD13	1.80	0.62
1:A:391:ARG:NH2	1:A:411:SER:O	2.33	0.62
1:D:3342:MET:HG3	1:D:3366:ALA:O	1.99	0.62
1:A:348:VAL:HG13	1:A:395:PRO:HB3	1.81	0.62
1:A:479:VAL:HG12	1:A:480:LYS:N	2.15	0.62
1:C:2518:MET:HG2	1:C:2521:LYS:HE2	1.81	0.62
1:D:3357:GLN:CD	1:D:3360:ARG:HG2	2.25	0.61
1:C:2438:THR:O	1:C:2441:LEU:CG	2.36	0.61
1:D:3433:ILE:HD12	1:D:3469:GLN:O	1.99	0.61
1:A:432:THR:HA	1:A:472:THR:O	2.00	0.61
1:A:467:PRO:HD3	1:B:1392:PHE:CE1	2.35	0.61
1:D:3562:HIS:O	1:D:3566:VAL:HG23	2.00	0.61
1:D:3342:MET:CG	1:D:3366:ALA:O	2.49	0.61
1:D:3432:THR:HG23	1:D:3471:ASN:HA	1.83	0.61
1:D:3422:VAL:HG13	1:D:3425:ASP:HB2	1.83	0.61
1:A:488:ARG:HH22	1:A:518:MET:HE3	1.66	0.60
1:C:2513:SER:CB	1:C:2540:SER:H	2.14	0.60
1:A:406:PRO:O	1:A:410:ILE:HB	2.02	0.60
1:D:3499:PRO:HD2	1:D:3530:ARG:NH1	2.17	0.60
1:B:1484:GLY:O	1:B:1488:ARG:HG3	2.02	0.60
1:D:3410:ILE:HG22	1:D:3412:LEU:H	1.67	0.60
1:B:1345:ALA:HB3	1:B:1364:PHE:H	1.67	0.60
1:B:1504:LEU:HD11	1:B:1527:MET:HE3	1.84	0.60
1:B:1391:ARG:O	1:B:1391:ARG:HG3	2.01	0.59
1:C:2440:GLY:C	1:C:2441:LEU:HD23	2.26	0.59
1:D:3582:VAL:HB	5:D:4054:HOH:O	2.00	0.59
1:A:439:TYR:H	1:A:493:ARG:NH1	1.95	0.59
1:C:2348:VAL:HA	1:C:2398:GLY:HA3	1.85	0.59
1:C:2419:ILE:HG22	1:C:2420:GLY:N	2.17	0.59
1:B:1433:ILE:HD12	1:B:1472:THR:HB	1.85	0.59
1:A:427:ALA:H	1:A:486:ARG:HH12	1.49	0.59
1:A:438:THR:O	1:A:438:THR:CG2	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2518:MET:CG	1:C:2521:LYS:HE2	2.33	0.59
1:A:464:GLU:C	1:A:466:MET:H	2.09	0.58
1:B:1421:PHE:HE1	1:B:1497:ARG:HD2	1.68	0.58
1:B:1434:ARG:NH2	1:B:1447:ASP:OD1	2.36	0.58
1:A:424:GLN:NE2	1:A:487:GLN:HA	2.19	0.58
1:D:3430:ALA:HB1	1:D:3435:GLU:HB3	1.84	0.58
1:B:1433:ILE:CD1	1:B:1472:THR:HB	2.33	0.58
1:C:2455:ASP:HA	1:D:3439:TYR:OH	2.04	0.58
1:C:2520:GLN:HG3	1:C:2538:ARG:NH1	2.18	0.58
1:D:3504:LEU:CD1	1:D:3527:MET:HE3	2.33	0.58
1:D:3441:LEU:CD1	1:D:3496:LEU:HD13	2.32	0.58
1:A:491:ILE:HG23	1:A:526:LEU:HD22	1.86	0.58
1:D:3514:GLU:C	1:D:3517:SER:H	2.12	0.58
1:C:2479:VAL:HG12	1:C:2480:LYS:N	2.18	0.57
1:C:2518:MET:HG2	1:C:2521:LYS:CE	2.34	0.57
1:D:3433:ILE:HD13	1:D:3463:VAL:HG13	1.86	0.57
1:C:2447:ASP:HB2	1:C:2470:LEU:CD1	2.34	0.57
1:D:3441:LEU:HB3	1:D:3445:TYR:CE1	2.39	0.57
1:D:3366:ALA:HA	1:D:3372:ILE:HD13	1.86	0.57
1:B:1526:LEU:HD22	1:B:1530:ARG:NH2	2.19	0.57
1:A:444:ASP:HB2	1:A:450:LEU:HD21	1.87	0.57
1:A:353:ASP:OD1	3:D:3600:ADP:H2'	2.04	0.57
1:D:3422:VAL:CG1	1:D:3490:ALA:CB	2.82	0.57
1:D:3437:LEU:HA	1:D:3493:ARG:HG2	1.85	0.57
1:C:2437:LEU:O	1:C:2496:LEU:HD23	2.05	0.56
1:A:498:ASN:HD22	1:A:530:ARG:NH2	2.02	0.56
2:A:601:ATP:O2'	1:D:3356:GLU:OE1	2.22	0.56
1:B:1342:MET:SD	1:B:1367:GLN:HG2	2.46	0.56
1:B:1447:ASP:CG	1:B:1470:LEU:HD21	2.30	0.56
1:C:2390:GLU:HG3	1:C:2503:MET:HE1	1.87	0.55
1:C:2518:MET:HG2	1:C:2521:LYS:HZ1	1.70	0.55
1:A:416:ARG:O	1:A:497:ARG:NH2	2.39	0.55
1:C:2538:ARG:HB2	1:C:2541:THR:OG1	2.06	0.55
1:A:473:GLU:O	1:A:479:VAL:HG23	2.07	0.55
1:B:1493:ARG:HH21	1:B:1497:ARG:HH21	1.53	0.55
1:D:3433:ILE:O	1:D:3437:LEU:HG	2.07	0.55
1:D:3405:GLN:NE2	1:D:3409:ASN:ND2	2.54	0.55
1:C:2445:TYR:O	1:C:2449:ASP:HB3	2.07	0.55
1:C:2479:VAL:HG12	1:C:2480:LYS:H	1.72	0.55
1:B:1514:GLU:O	1:B:1518:MET:HG3	2.07	0.55
1:C:2415:TRP:NE1	1:C:2419:ILE:HD11	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3359:LEU:HD22	1:D:3362:ILE:HD12	1.88	0.55
1:C:2433:ILE:HD12	1:C:2466:MET:HE1	1.89	0.54
1:C:2518:MET:HA	1:C:2521:LYS:CG	2.36	0.54
1:D:3371:ILE:HG22	1:D:3372:ILE:N	2.21	0.54
1:D:3407:ILE:C	1:D:3409:ASN:H	2.15	0.54
1:A:372:ILE:O	1:A:372:ILE:HG13	2.07	0.54
1:C:2381:GLY:HA2	2:C:2601:ATP:O2A	2.07	0.54
1:A:407:ILE:HG13	1:A:408:ASP:N	2.22	0.54
1:D:3439:TYR:O	1:D:3440:GLY:C	2.51	0.54
1:A:367:GLN:O	1:A:370:SER:OG	2.24	0.53
1:B:1421:PHE:O	1:B:1503:MET:HB2	2.08	0.53
1:C:2428:ILE:HG12	1:C:2486:ARG:HH12	1.73	0.53
1:C:2446:THR:CG2	1:C:2447:ASP:N	2.71	0.53
1:A:523:LEU:O	1:A:527:MET:HG3	2.08	0.53
1:B:1469:GLN:O	1:B:1470:LEU:HB3	2.08	0.53
1:D:3419:ILE:CG1	1:D:3499:PRO:HG2	2.38	0.53
1:D:3438:THR:CG2	1:D:3438:THR:O	2.56	0.53
1:B:1498:ASN:N	1:B:1499:PRO:HD3	2.24	0.53
1:D:3459:ALA:HA	1:D:3462:PHE:CE1	2.43	0.53
1:B:1459:ALA:O	1:B:1463:VAL:HG23	2.09	0.53
1:A:391:ARG:NH2	1:A:407:ILE:O	2.39	0.53
1:B:1419:ILE:CG2	1:B:1501:ILE:HD12	2.38	0.53
1:D:3431:GLY:C	1:D:3473:GLU:HA	2.34	0.53
1:D:3481:ILE:HG22	1:D:3483:GLY:H	1.74	0.53
1:C:2424:GLN:CG	1:C:2425:ASP:H	2.21	0.53
1:A:421:PHE:C	1:A:421:PHE:CD2	2.87	0.52
1:D:3390:GLU:CG	1:D:3503:MET:HE1	2.38	0.52
1:C:2518:MET:HA	1:C:2521:LYS:CD	2.40	0.52
1:A:415:TRP:NE1	1:A:419:ILE:HD11	2.24	0.52
1:B:1429:MET:SD	1:B:1493:ARG:NH1	2.83	0.52
1:B:1432:THR:HB	1:B:1435:GLU:HB2	1.92	0.52
1:C:2355:SER:O	1:C:2356:GLU:HB2	2.10	0.52
1:C:2372:ILE:HG12	1:C:2533:LEU:HB3	1.92	0.52
1:D:3442:GLU:HB2	1:D:3445:TYR:CZ	2.45	0.52
1:B:1421:PHE:CD2	1:B:1502:LEU:HD12	2.45	0.51
1:B:1345:ALA:O	1:B:1363:SER:HA	2.10	0.51
1:A:423:SER:OG	1:A:505:ASP:HB3	2.11	0.51
1:A:419:ILE:HG22	1:A:420:GLY:N	2.26	0.51
1:A:427:ALA:CB	1:A:486:ARG:NH1	2.68	0.51
1:A:491:ILE:O	1:A:494:ALA:HB3	2.11	0.51
1:D:3422:VAL:HG22	1:D:3425:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3428:ILE:HD12	1:D:3493:ARG:HH12	1.76	0.51
1:D:3512:ASP:O	1:D:3515:SER:N	2.41	0.51
1:D:3405:GLN:NE2	1:D:3409:ASN:HD21	2.09	0.51
1:A:439:TYR:HB2	1:A:493:ARG:HH22	1.75	0.51
1:B:1424:GLN:HE22	1:B:1493:ARG:CZ	2.25	0.50
1:C:2428:ILE:HG12	1:C:2486:ARG:NH1	2.27	0.50
1:D:3419:ILE:HG12	1:D:3499:PRO:HG2	1.94	0.50
1:B:1349:ASP:HB2	1:B:1397:ALA:HB3	1.93	0.50
1:C:2421:PHE:C	1:C:2421:PHE:CD2	2.89	0.50
1:D:3422:VAL:HG11	1:D:3490:ALA:HB1	1.92	0.50
1:A:467:PRO:C	1:A:469:GLN:H	2.20	0.50
1:C:2443:GLY:O	1:C:2444:ASP:HB2	2.12	0.50
1:D:3347:HIS:H	1:D:3363:SER:HB3	1.75	0.50
1:A:479:VAL:HG13	1:B:1392:PHE:HB3	1.92	0.50
1:C:2345:ALA:O	1:C:2363:SER:HA	2.11	0.50
1:D:3422:VAL:CB	1:D:3490:ALA:CB	2.89	0.50
1:B:1521:LYS:O	1:B:1524:ASP:HB2	2.12	0.50
1:A:565:LEU:HB3	1:A:572:TYR:CD2	2.46	0.50
1:B:1473:GLU:O	1:B:1479:VAL:HB	2.12	0.50
1:B:1348:VAL:O	1:B:1360:ARG:O	2.29	0.49
1:D:3514:GLU:O	1:D:3517:SER:N	2.44	0.49
1:A:421:PHE:C	1:A:421:PHE:HD2	2.21	0.49
1:D:3427:ALA:HB2	1:D:3486:ARG:NH1	2.27	0.49
1:B:1441:LEU:O	1:B:1442:GLU:HB2	2.12	0.49
1:D:3345:ALA:O	1:D:3363:SER:HA	2.13	0.49
1:D:3439:TYR:O	1:D:3441:LEU:HG	2.12	0.49
1:C:2447:ASP:HB2	1:C:2470:LEU:HD12	1.95	0.49
1:A:419:ILE:CG2	1:A:503:MET:HE2	2.42	0.49
1:C:2542:ILE:HG23	1:C:2548:ILE:HG12	1.94	0.49
1:C:2562:HIS:O	1:C:2566:VAL:HG23	2.13	0.49
1:D:3421:PHE:CZ	1:D:3424:GLN:NE2	2.78	0.49
1:C:2432:THR:HG22	1:C:2433:ILE:N	2.28	0.48
1:C:2446:THR:CG2	1:C:2447:ASP:H	2.25	0.48
1:A:448:GLU:OE2	1:A:452:GLN:NE2	2.46	0.48
1:B:1493:ARG:NH2	1:B:1497:ARG:NH2	2.61	0.48
1:D:3432:THR:HG22	1:D:3434:ARG:HB3	1.96	0.48
1:A:444:ASP:O	1:A:445:TYR:CD2	2.66	0.48
1:A:517:SER:O	1:A:520:GLN:HB2	2.13	0.48
1:C:2481:ILE:HG22	1:C:2482:SER:O	2.13	0.48
1:B:1515:SER:HA	1:B:1518:MET:HE3	1.94	0.48
1:C:2446:THR:HG22	1:C:2447:ASP:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1515:SER:O	1:B:1519:VAL:HB	2.14	0.48
1:C:2505:ASP:HB3	1:C:2535:ILE:HB	1.95	0.48
1:C:2526:LEU:O	1:C:2530:ARG:HD2	2.14	0.48
1:A:517:SER:CB	5:A:4065:HOH:O	2.61	0.48
1:B:1429:MET:HE1	1:B:1436:ASN:O	2.14	0.48
1:D:3488:ARG:C	1:D:3490:ALA:H	2.19	0.48
1:C:2520:GLN:HG3	1:C:2538:ARG:HH12	1.78	0.47
1:D:3520:GLN:O	1:D:3524:ASP:CG	2.57	0.47
1:D:3347:HIS:O	1:D:3398:GLY:HA3	2.14	0.47
1:A:352:TYR:HD2	1:A:358:ILE:HG13	1.78	0.47
1:D:3402:ILE:C	1:D:3404:GLY:N	2.72	0.47
1:A:459:ALA:C	1:A:461:SER:H	2.21	0.47
1:B:1386:PHE:CE1	1:B:1504:LEU:O	2.63	0.47
1:B:1446:THR:HB	1:B:1449:ASP:HB2	1.96	0.47
1:C:2384:THR:OG1	2:C:2601:ATP:O2A	2.26	0.47
1:C:2419:ILE:HG22	1:C:2420:GLY:H	1.80	0.47
1:A:485:GLN:NE2	1:B:1416:ARG:HH11	2.11	0.47
1:A:350:PHE:HA	1:A:396:THR:HG23	1.96	0.47
1:C:2455:ASP:CA	1:D:3439:TYR:OH	2.63	0.47
1:A:542:ILE:HD12	1:A:580:LEU:HD21	1.96	0.47
1:B:1441:LEU:O	1:B:1442:GLU:CB	2.63	0.47
1:C:2421:PHE:HD2	1:C:2422:VAL:N	2.13	0.47
1:C:2424:GLN:CG	1:C:2425:ASP:N	2.78	0.47
1:C:2479:VAL:CG1	1:C:2480:LYS:H	2.27	0.47
1:D:3370:SER:CB	1:D:3546:ASP:OD2	2.55	0.47
1:D:3488:ARG:C	1:D:3490:ALA:N	2.71	0.47
1:B:1481:ILE:HG13	1:B:1486:ARG:HH21	1.80	0.47
1:D:3409:ASN:C	1:D:3410:ILE:HG13	2.39	0.47
1:A:394:GLN:OE1	1:A:408:ASP:OD2	2.33	0.46
1:C:2347:HIS:ND1	1:C:2361:ASP:OD2	2.48	0.46
1:C:2377:PRO:HG3	1:C:2579:GLN:HE22	1.80	0.46
1:D:3407:ILE:O	1:D:3407:ILE:HG22	2.14	0.46
1:A:475:GLY:O	1:A:477:ARG:N	2.48	0.46
1:C:2449:ASP:OD1	1:C:2449:ASP:C	2.59	0.46
1:C:2518:MET:CA	1:C:2521:LYS:HG2	2.44	0.46
1:D:3492:ALA:O	1:D:3495:PHE:HB2	2.16	0.46
1:C:2527:MET:HE2	1:C:2532:THR:HG21	1.98	0.46
1:D:3366:ALA:HA	1:D:3372:ILE:CD1	2.46	0.46
1:D:3449:ASP:O	1:D:3452:GLN:HB2	2.15	0.46
1:D:3371:ILE:CG2	1:D:3372:ILE:N	2.79	0.46
1:B:1432:THR:HG22	1:B:1434:ARG:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2446:THR:O	1:C:2449:ASP:CG	2.54	0.46
1:C:2451:TRP:CH2	1:C:2464:GLU:HG3	2.50	0.46
1:C:2497:ARG:NH1	5:C:4049:HOH:O	2.48	0.46
1:D:3504:LEU:HD11	1:D:3527:MET:HE3	1.97	0.45
1:A:345:ALA:O	1:A:363:SER:HA	2.17	0.45
1:A:380:GLY:N	2:A:601:ATP:O1B	2.50	0.45
1:B:1502:LEU:HD23	1:B:1532:THR:HG23	1.98	0.45
1:D:3498:ASN:N	1:D:3499:PRO:HD3	2.32	0.45
1:A:418:GLN:HE21	1:A:418:GLN:HB3	1.57	0.45
1:C:2390:GLU:OE1	1:C:2421:PHE:HD1	2.00	0.45
1:D:3422:VAL:CG1	1:D:3490:ALA:HB1	2.46	0.45
1:D:3447:ASP:OD2	1:D:3470:LEU:HD12	2.17	0.45
1:A:424:GLN:HE22	1:A:487:GLN:HA	1.82	0.45
1:C:2491:ILE:HG23	1:C:2526:LEU:HD22	1.98	0.45
1:D:3514:GLU:HA	1:D:3517:SER:OG	2.17	0.45
1:A:349:ASP:HB2	1:A:397:ALA:HB3	1.98	0.45
1:B:1447:ASP:O	1:B:1451:TRP:CD1	2.70	0.44
1:A:458:PHE:HD2	1:A:458:PHE:N	2.15	0.44
1:B:1502:LEU:HD13	1:B:1530:ARG:NH2	2.33	0.44
1:D:3400:ILE:O	1:D:3407:ILE:HG13	2.17	0.44
1:C:2580:LEU:HD23	1:C:2580:LEU:HA	1.83	0.44
1:D:3441:LEU:HA	1:D:3441:LEU:HD23	1.53	0.44
1:A:458:PHE:N	1:A:458:PHE:CD2	2.86	0.44
1:B:1352:TYR:CD1	1:B:1358:ILE:HD12	2.52	0.44
1:C:2421:PHE:CE2	1:C:2423:SER:HB3	2.52	0.44
1:C:2366:ALA:HB2	1:C:2372:ILE:HD13	1.99	0.44
1:C:2509:ALA:HA	5:C:4070:HOH:O	2.17	0.44
1:B:1446:THR:O	1:B:1450:LEU:HG	2.17	0.44
1:C:2479:VAL:CG1	1:C:2480:LYS:N	2.80	0.44
1:B:1343:LEU:HD12	1:B:1501:ILE:HD13	1.99	0.44
1:C:2410:ILE:H	1:C:2410:ILE:HG13	1.59	0.44
1:D:3376:GLY:HA2	1:D:3550:PHE:HE1	1.82	0.44
1:B:1434:ARG:O	1:B:1438:THR:HB	2.18	0.44
1:B:1434:ARG:HH11	1:B:1434:ARG:CG	2.30	0.44
1:C:2432:THR:HG22	1:C:2434:ARG:H	1.83	0.44
1:D:3513:SER:O	1:D:3517:SER:N	2.51	0.44
1:C:2407:ILE:HA	1:C:2410:ILE:HD12	1.99	0.43
1:C:2455:ASP:OD1	1:D:3439:TYR:OH	2.35	0.43
1:D:3374:PHE:O	1:D:3382:LYS:HG2	2.19	0.43
1:A:366:ALA:HB2	1:A:372:ILE:HD13	2.00	0.43
1:A:415:TRP:CE2	1:A:419:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1424:GLN:HE22	1:B:1493:ARG:NE	2.17	0.43
1:B:1388:LEU:HD23	1:B:1393:TYR:HB2	2.01	0.43
1:B:1419:ILE:HG22	1:B:1501:ILE:HD12	2.01	0.43
1:C:2421:PHE:C	1:C:2421:PHE:HD2	2.26	0.43
1:D:3483:GLY:O	1:D:3487:GLN:HG3	2.19	0.43
1:A:366:ALA:HB2	1:A:372:ILE:CD1	2.49	0.43
1:B:1525:SER:HA	1:B:1528:LYS:HD2	2.00	0.43
1:D:3434:ARG:HH12	1:D:3445:TYR:C	2.27	0.43
1:A:480:LYS:NZ	1:B:1412:LEU:HD22	2.33	0.43
1:D:3451:TRP:HZ3	1:D:3460:ARG:O	2.01	0.43
1:B:1406:PRO:HB2	1:B:1409:ASN:ND2	2.34	0.42
1:C:2518:MET:C	1:C:2521:LYS:HG2	2.44	0.42
1:D:3425:ASP:O	1:D:3426:SER:O	2.36	0.42
1:D:3359:LEU:HD22	1:D:3362:ILE:CD1	2.49	0.42
1:A:488:ARG:HA	1:A:491:ILE:HD12	2.00	0.42
1:B:1542:ILE:HD12	1:B:1580:LEU:HD21	2.00	0.42
1:C:2577:SER:O	1:C:2581:THR:HB	2.19	0.42
1:D:3489:LEU:O	1:D:3492:ALA:HB3	2.20	0.42
1:C:2383:SER:HB2	2:C:2601:ATP:O1A	2.20	0.42
1:D:3476:GLU:H	1:D:3476:GLU:HG3	1.55	0.42
1:D:3430:ALA:HB3	1:D:3436:ASN:CG	2.45	0.42
1:C:2376:GLY:HA3	1:C:2551:ILE:O	2.20	0.41
1:A:454:LEU:O	1:A:459:ALA:N	2.51	0.41
1:D:3357:GLN:NE2	1:D:3360:ARG:HG2	2.35	0.41
1:D:3394:GLN:OE1	1:D:3394:GLN:HA	2.19	0.41
1:D:3488:ARG:HE	1:D:3488:ARG:HB2	1.59	0.41
1:D:3425:ASP:O	1:D:3426:SER:C	2.64	0.41
1:A:459:ALA:C	1:A:461:SER:N	2.79	0.41
1:B:1433:ILE:HD11	1:B:1472:THR:HB	2.03	0.41
1:D:3432:THR:HA	1:D:3472:THR:O	2.21	0.41
1:D:3535:ILE:HG22	1:D:3537:HIS:CE1	2.56	0.41
1:A:479:VAL:CG1	1:A:480:LYS:H	2.30	0.41
1:A:538:ARG:O	1:A:541:THR:HB	2.21	0.41
1:C:2402:ILE:HD12	1:C:2501:ILE:HD11	2.02	0.41
1:D:3467:PRO:O	1:D:3468:ASP:HB2	2.20	0.41
1:A:430:ALA:HB1	1:A:476:GLU:OE2	2.20	0.41
1:B:1534:VAL:HG12	1:B:1535:ILE:N	2.35	0.41
1:C:2409:ASN:HD22	1:C:2409:ASN:HA	1.62	0.41
1:C:2455:ASP:C	1:D:3439:TYR:OH	2.64	0.41
1:D:3407:ILE:HG21	1:D:3414:ASN:ND2	2.36	0.41
1:C:2375:ALA:HB1	1:C:2575:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2409:ASN:O	1:C:2411:SER:N	2.53	0.41
1:C:2446:THR:HG23	1:C:2447:ASP:H	1.84	0.41
1:C:2481:ILE:HG23	1:C:2485:GLN:HB2	2.02	0.41
1:D:3421:PHE:CD2	1:D:3421:PHE:N	2.89	0.41
1:D:3468:ASP:HB3	1:D:3471:ASN:HB2	2.02	0.41
1:D:3518:MET:HE3	1:D:3518:MET:HB2	2.00	0.41
1:A:451:TRP:CH2	1:A:464:GLU:HG3	2.56	0.41
1:C:2462:PHE:O	1:C:2466:MET:HG3	2.20	0.41
1:D:3367:GLN:O	1:D:3531:THR:HG23	2.21	0.41
1:C:2444:ASP:OD1	1:C:2444:ASP:N	2.54	0.40
1:C:2572:TYR:HE1	1:C:2576:VAL:HG21	1.86	0.40
1:D:3442:GLU:HB3	1:D:3443:GLY:H	1.20	0.40
1:D:3459:ALA:HA	1:D:3462:PHE:CD1	2.56	0.40
1:C:2419:ILE:CG2	1:C:2420:GLY:N	2.83	0.40
1:D:3430:ALA:HB1	1:D:3435:GLU:CB	2.50	0.40
1:D:3434:ARG:O	1:D:3438:THR:HB	2.22	0.40
1:D:3473:GLU:O	1:D:3479:VAL:HB	2.21	0.40
1:A:498:ASN:ND2	1:A:530:ARG:NH2	2.69	0.40
1:A:562:HIS:O	1:A:566:VAL:HG23	2.21	0.40
1:C:2449:ASP:OD1	1:C:2450:LEU:HG	2.21	0.40
1:C:2581:THR:HG22	1:C:2582:VAL:HG23	2.03	0.40
1:D:3462:PHE:HD2	1:D:3485:GLN:CD	2.30	0.40
1:B:1358:ILE:HD13	3:B:1600:ADP:H1'	2.02	0.40
1:B:1491:ILE:HG23	1:B:1526:LEU:HG	2.03	0.40
1:C:2443:GLY:O	1:C:2444:ASP:CB	2.69	0.40
1:C:2458:PHE:HA	1:D:3439:TYR:CE2	2.56	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	240/243 (99%)	198 (82%)	27 (11%)	15 (6%)	1	6
1	B	240/243 (99%)	200 (83%)	29 (12%)	11 (5%)	2	12
1	C	240/243 (99%)	202 (84%)	22 (9%)	16 (7%)	1	6
1	D	239/243 (98%)	189 (79%)	34 (14%)	16 (7%)	1	6
All	All	959/972 (99%)	789 (82%)	112 (12%)	58 (6%)	1	7

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	LEU
1	A	426	SER
1	A	444	ASP
1	A	467	PRO
1	A	476	GLU
1	A	516	GLU
1	B	1347	HIS
1	B	1425	ASP
1	B	1498	ASN
1	C	2410	ILE
1	C	2426	SER
1	C	2427	ALA
1	C	2460	ARG
1	C	2467	PRO
1	C	2469	GLN
1	C	2528	LYS
1	C	2553	LYS
1	D	3354	ASP
1	D	3369	ASN
1	D	3395	PRO
1	D	3406	PRO
1	D	3408	ASP
1	D	3423	SER
1	D	3426	SER
1	D	3469	GLN
1	A	513	SER
1	A	553	LYS
1	B	1439	TYR
1	B	1442	GLU
1	B	1499	PRO
1	C	2398	GLY
1	C	2425	ASP
1	C	2513	SER

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Mol	Chain	Res	Type
1	D	3440	GLY
1	D	3508	THR
1	D	3513	SER
1	A	483	GLY
1	A	510	SER
1	A	578	GLU
1	B	1469	GLN
1	B	1480	LYS
1	C	2356	GLU
1	C	2439	TYR
1	C	2446	THR
1	D	3361	ASP
1	D	3507	ALA
1	A	458	PHE
1	B	1428	ILE
1	C	2355	SER
1	D	3347	HIS
1	D	3409	ASN
1	D	3511	LEU
1	A	361	ASP
1	A	413	GLU
1	A	425	ASP
1	B	1460	ARG
1	C	2444	ASP
1	B	1467	PRO

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	196/204 (96%)	176 (90%)	20 (10%)	7	28
1	B	202/204 (99%)	183 (91%)	19 (9%)	8	31
1	C	195/204 (96%)	182 (93%)	13 (7%)	15	43
1	D	201/204 (98%)	184 (92%)	17 (8%)	10	35
All	All	794/816 (97%)	725 (91%)	69 (9%)	9	34

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	LEU
1	A	349	ASP
1	A	360	ARG
1	A	368	PRO
1	A	388	LEU
1	A	401	THR
1	A	406	PRO
1	A	408	ASP
1	A	410	ILE
1	A	418	GLN
1	A	421	PHE
1	A	424	GLN
1	A	448	GLU
1	A	453	VAL
1	A	458	PHE
1	A	461	SER
1	A	467	PRO
1	A	476	GLU
1	A	530	ARG
1	A	559	SER
1	B	1344	SER
1	B	1361	ASP
1	B	1382	LYS
1	B	1391	ARG
1	B	1394	GLN
1	B	1406	PRO
1	B	1429	MET
1	B	1434	ARG
1	B	1438	THR
1	B	1446	THR
1	B	1458	PHE
1	B	1463	VAL
1	B	1481	ILE
1	B	1515	SER
1	B	1527	MET
1	B	1535	ILE
1	B	1548	ILE
1	B	1570	PRO
1	B	1581	THR
1	C	2343	LEU
1	C	2372	ILE
1	C	2426	SER

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Mol	Chain	Res	Type
1	C	2437	LEU
1	C	2442	GLU
1	C	2448	GLU
1	C	2460	ARG
1	C	2467	PRO
1	C	2468	ASP
1	C	2504	LEU
1	C	2533	LEU
1	C	2539	LEU
1	C	2570	PRO
1	D	3344	SER
1	D	3362	ILE
1	D	3368	PRO
1	D	3377	PRO
1	D	3382	LYS
1	D	3401	THR
1	D	3406	PRO
1	D	3419	ILE
1	D	3437	LEU
1	D	3438	THR
1	D	3442	GLU
1	D	3467	PRO
1	D	3476	GLU
1	D	3489	LEU
1	D	3513	SER
1	D	3523	LEU
1	D	3533	LEU

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

Mol	Chain	Res	Type
1	A	369	ASN
1	A	394	GLN
1	A	418	GLN
1	A	498	ASN
1	B	1465	ASN
1	B	1471	ASN
1	B	1485	GLN
1	B	1498	ASN
1	C	2394	GLN
1	C	2409	ASN
1	C	2537	HIS

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Mol	Chain	Res	Type
1	D	3405	GLN
1	D	3424	GLN
1	D	3436	ASN
1	D	3569	HIS
1	D	3579	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	B	1600	-	28,29,29	2.29	8 (28%)	43,45,45	1.81	8 (18%)
3	ADP	D	3600	4	28,29,29	2.04	8 (28%)	43,45,45	2.02	9 (20%)
2	ATP	A	601	-	32,33,33	2.64	13 (40%)	48,52,52	3.17	17 (35%)
2	ATP	C	2601	-	32,33,33	2.70	13 (40%)	48,52,52	2.92	16 (33%)

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	B	1600	-	-	2/16/32/32	0/3/3/3
3	ADP	D	3600	4	-	1/16/32/32	0/3/3/3
2	ATP	A	601	-	-	4/22/38/38	0/3/3/3
2	ATP	C	2601	-	-	4/22/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2601	ATP	PA-O3A	-7.81	1.51	1.59
3	B	1600	ADP	PA-O3A	-7.32	1.51	1.59
2	A	601	ATP	PA-O3A	-6.75	1.52	1.59
2	A	601	ATP	PB-O3B	-6.52	1.52	1.59
2	C	2601	ATP	PB-O3B	-6.44	1.52	1.59
3	D	3600	ADP	PA-O3A	-6.36	1.52	1.59
2	C	2601	ATP	O5'-C5'	-5.27	1.24	1.44
3	B	1600	ADP	C5-N7	-5.15	1.29	1.39
2	A	601	ATP	PB-O3A	4.61	1.64	1.59
2	A	601	ATP	C4-N3	4.39	1.42	1.34
2	A	601	ATP	O5'-C5'	-4.15	1.28	1.44
2	C	2601	ATP	PA-O5'	-4.00	1.43	1.59
2	C	2601	ATP	PB-O3A	3.36	1.63	1.59
3	B	1600	ADP	C4-N9	-3.30	1.30	1.37
2	C	2601	ATP	PB-O2B	-3.11	1.40	1.55
2	C	2601	ATP	C4-N9	-3.08	1.31	1.37
2	A	601	ATP	PA-O5'	-3.06	1.47	1.59
3	D	3600	ADP	PB-O3B	-3.06	1.43	1.54
3	D	3600	ADP	PA-O2A	-3.04	1.41	1.55
3	D	3600	ADP	PB-O1B	-2.97	1.41	1.50
3	D	3600	ADP	C5-N7	-2.94	1.33	1.39
3	B	1600	ADP	PA-O2A	-2.92	1.41	1.55
3	B	1600	ADP	PB-O3B	-2.84	1.44	1.54
2	A	601	ATP	O4'-C1'	2.73	1.48	1.42
2	A	601	ATP	PA-O2A	-2.71	1.42	1.55
2	A	601	ATP	PB-O2B	-2.71	1.42	1.55
2	C	2601	ATP	C4-N3	2.67	1.39	1.34
3	B	1600	ADP	C8-N9	-2.67	1.33	1.37
2	C	2601	ATP	O4'-C1'	2.66	1.48	1.42
2	A	601	ATP	C3'-C4'	-2.62	1.46	1.53
2	A	601	ATP	C5-N7	-2.56	1.34	1.39
2	C	2601	ATP	PA-O2A	-2.55	1.43	1.55
3	D	3600	ADP	C4-N9	-2.50	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2601	ATP	C5-C4	-2.35	1.34	1.39
2	C	2601	ATP	C5-N7	-2.32	1.34	1.39
3	B	1600	ADP	PB-O1B	-2.32	1.43	1.50
2	C	2601	ATP	PA-O1A	-2.31	1.42	1.50
2	A	601	ATP	PB-O1B	-2.30	1.42	1.50
3	D	3600	ADP	PA-O1A	-2.28	1.42	1.50
3	B	1600	ADP	O3'-C3'	2.27	1.48	1.43
3	D	3600	ADP	PB-O2B	-2.25	1.46	1.54
2	A	601	ATP	C5'-C4'	-2.12	1.45	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ATP	O5'-C5'-C4'	12.31	150.90	108.99
2	C	2601	ATP	O5'-C5'-C4'	11.18	147.06	108.99
2	A	601	ATP	O3A-PB-O1B	-7.48	88.20	110.70
2	C	2601	ATP	O3A-PB-O1B	-6.90	89.93	110.70
2	C	2601	ATP	PA-O5'-C5'	6.38	157.93	121.35
2	A	601	ATP	PA-O5'-C5'	6.29	157.40	121.35
3	D	3600	ADP	N3-C2-N1	-6.14	119.29	128.58
2	C	2601	ATP	O5'-PA-O1A	-6.14	84.60	108.94
2	A	601	ATP	C5'-C4'-C3'	-6.06	93.40	115.21
2	A	601	ATP	O5'-PA-O1A	-6.00	85.16	108.94
3	B	1600	ADP	N3-C2-N1	-5.95	119.57	128.58
3	D	3600	ADP	C5-C4-N3	-5.46	119.19	126.72
2	C	2601	ATP	O2A-PA-O3A	5.18	121.27	107.27
2	A	601	ATP	O2A-PA-O3A	4.92	120.58	107.27
2	A	601	ATP	O4'-C4'-C3'	4.85	114.78	105.15
3	B	1600	ADP	C5-C4-N3	-4.77	120.16	126.72
2	C	2601	ATP	O4'-C4'-C3'	4.67	114.42	105.15
2	C	2601	ATP	C5'-C4'-C3'	-4.62	98.57	115.21
3	D	3600	ADP	C2-N3-C4	4.51	122.84	111.83
2	A	601	ATP	O2B-PB-O3B	4.40	119.17	107.27
2	A	601	ATP	O2B-PB-O3A	-4.15	96.05	107.27
3	D	3600	ADP	N3-C4-N9	4.14	134.20	127.17
3	B	1600	ADP	C2-N3-C4	4.08	121.79	111.83
2	C	2601	ATP	O2B-PB-O3B	3.59	116.99	107.27
3	D	3600	ADP	N9-C8-N7	-3.49	108.99	113.94
3	B	1600	ADP	N3-C4-N9	3.25	132.69	127.17
3	D	3600	ADP	C4-N9-C8	3.22	109.11	105.74
2	A	601	ATP	C4-C5-N7	3.15	114.19	110.58
2	C	2601	ATP	O3B-PB-O1B	2.96	119.61	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ATP	C3'-C2'-C1'	2.82	106.80	101.46
3	D	3600	ADP	O3B-PB-O3A	2.82	114.09	104.64
3	B	1600	ADP	N9-C8-N7	-2.75	110.04	113.94
3	B	1600	ADP	C5-N7-C8	2.71	107.71	103.45
2	C	2601	ATP	O2A-PA-O5'	-2.65	95.54	107.57
3	B	1600	ADP	C4-C5-N7	-2.64	107.56	110.58
2	A	601	ATP	O3'-C3'-C4'	2.53	118.36	111.08
2	C	2601	ATP	C3'-C2'-C1'	2.49	106.18	101.46
2	C	2601	ATP	O2A-PA-O1A	2.47	123.93	112.44
2	C	2601	ATP	C4-C5-N7	2.44	113.38	110.58
2	C	2601	ATP	O2B-PB-O3A	-2.44	100.67	107.27
2	A	601	ATP	O4'-C4'-C5'	-2.41	101.62	109.33
3	D	3600	ADP	C5-N7-C8	2.40	107.22	103.45
2	C	2601	ATP	O2B-PB-O1B	2.33	123.31	112.44
2	A	601	ATP	O2B-PB-O1B	2.32	123.26	112.44
2	A	601	ATP	O2A-PA-O1A	2.26	122.95	112.44
3	D	3600	ADP	C4-C5-N7	-2.25	108.01	110.58
2	A	601	ATP	O3B-PB-O1B	2.11	117.06	110.70
2	C	2601	ATP	O4'-C4'-C5'	-2.09	102.65	109.33
3	B	1600	ADP	C2-N1-C6	2.03	122.06	118.73
2	A	601	ATP	O2A-PA-O5'	-2.02	98.39	107.57

There are no chirality outliers.

All (11) torsion outliers are listed below:

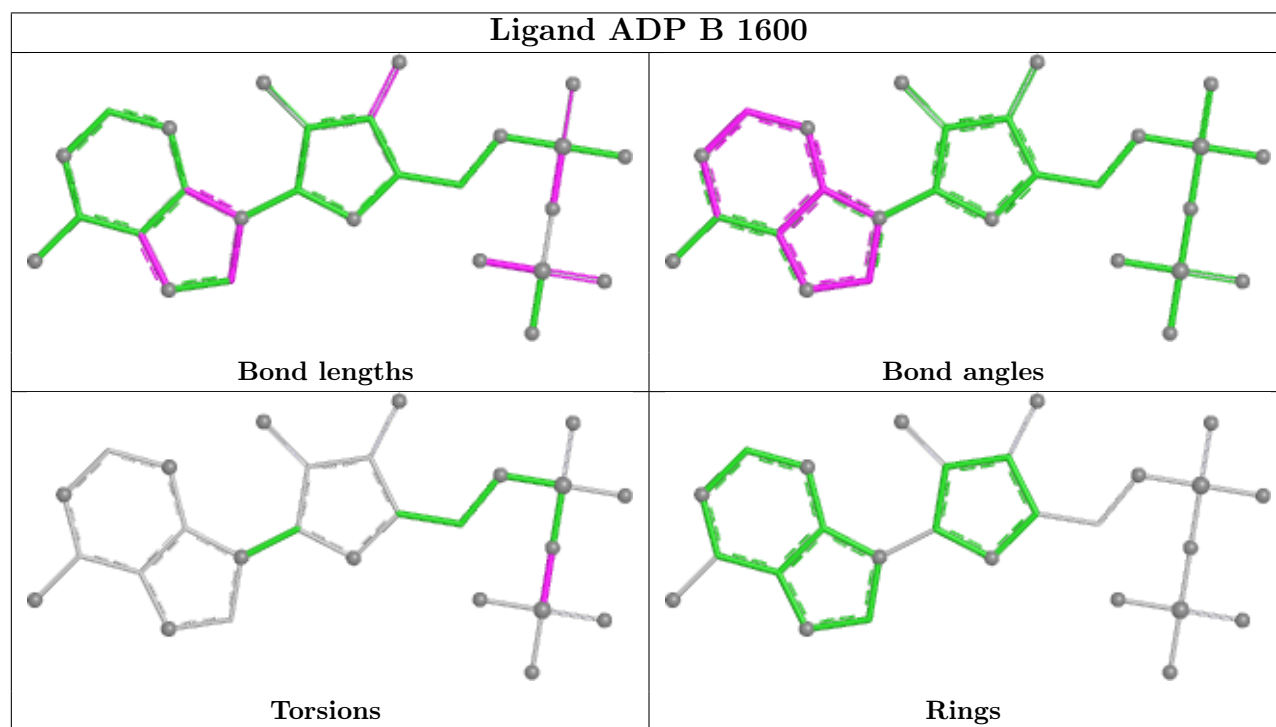
Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C4'-C5'-O5'-PA
2	C	2601	ATP	C4'-C5'-O5'-PA
2	C	2601	ATP	PB-O3B-PG-O3G
2	A	601	ATP	PG-O3B-PB-O2B
2	A	601	ATP	PA-O3A-PB-O2B
2	C	2601	ATP	PG-O3B-PB-O2B
3	B	1600	ADP	PA-O3A-PB-O1B
3	B	1600	ADP	PA-O3A-PB-O3B
3	D	3600	ADP	PA-O3A-PB-O3B
2	A	601	ATP	PA-O3A-PB-O1B
2	C	2601	ATP	PA-O3A-PB-O2B

There are no ring outliers.

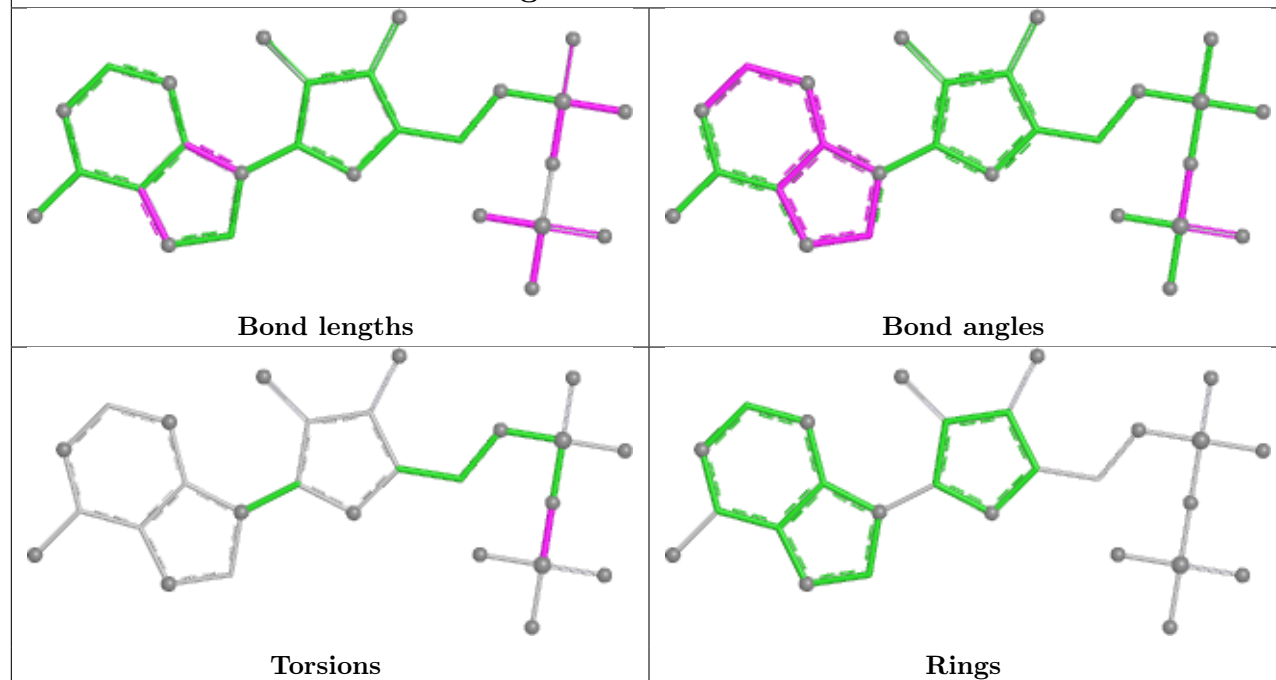
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1600	ADP	2	0
3	D	3600	ADP	1	0
2	A	601	ATP	2	0
2	C	2601	ATP	3	0

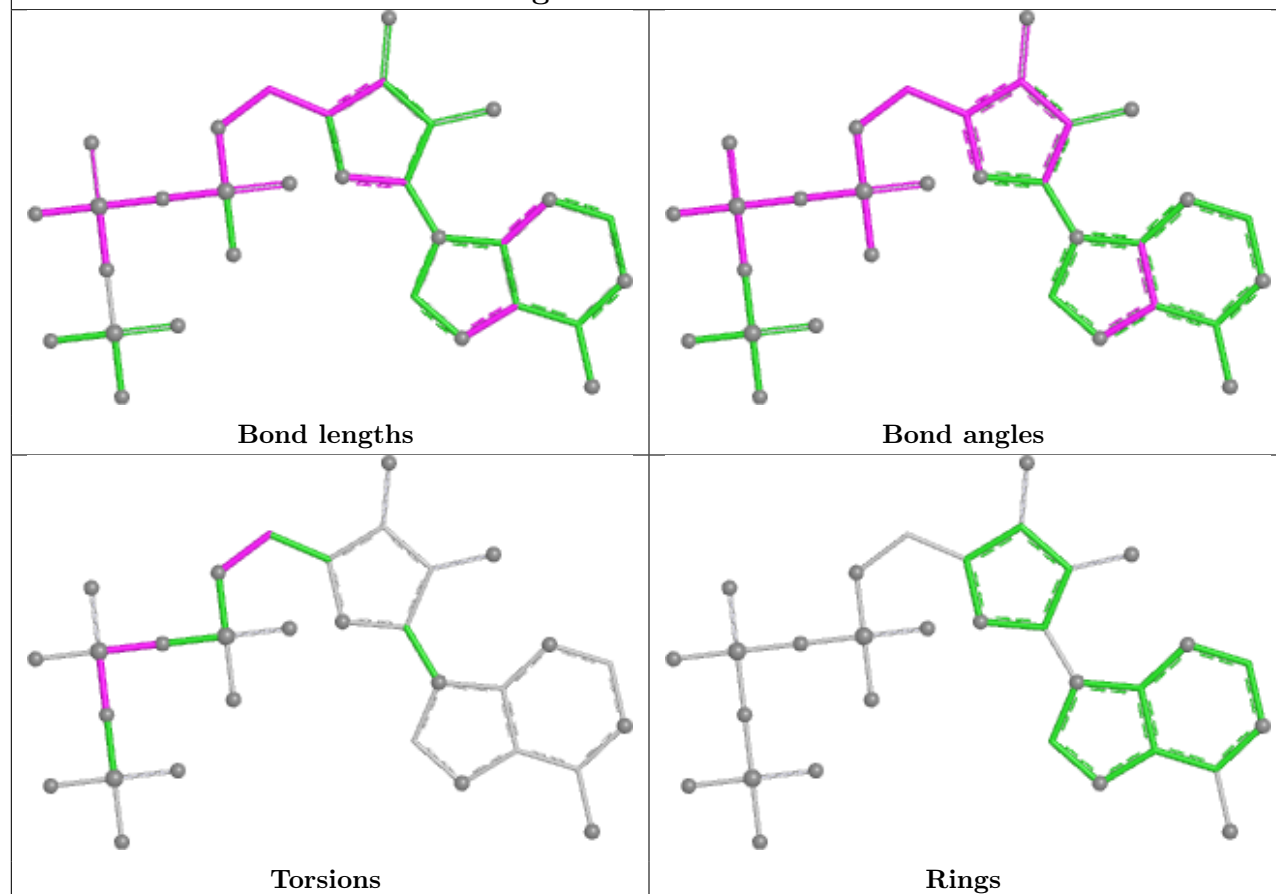
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

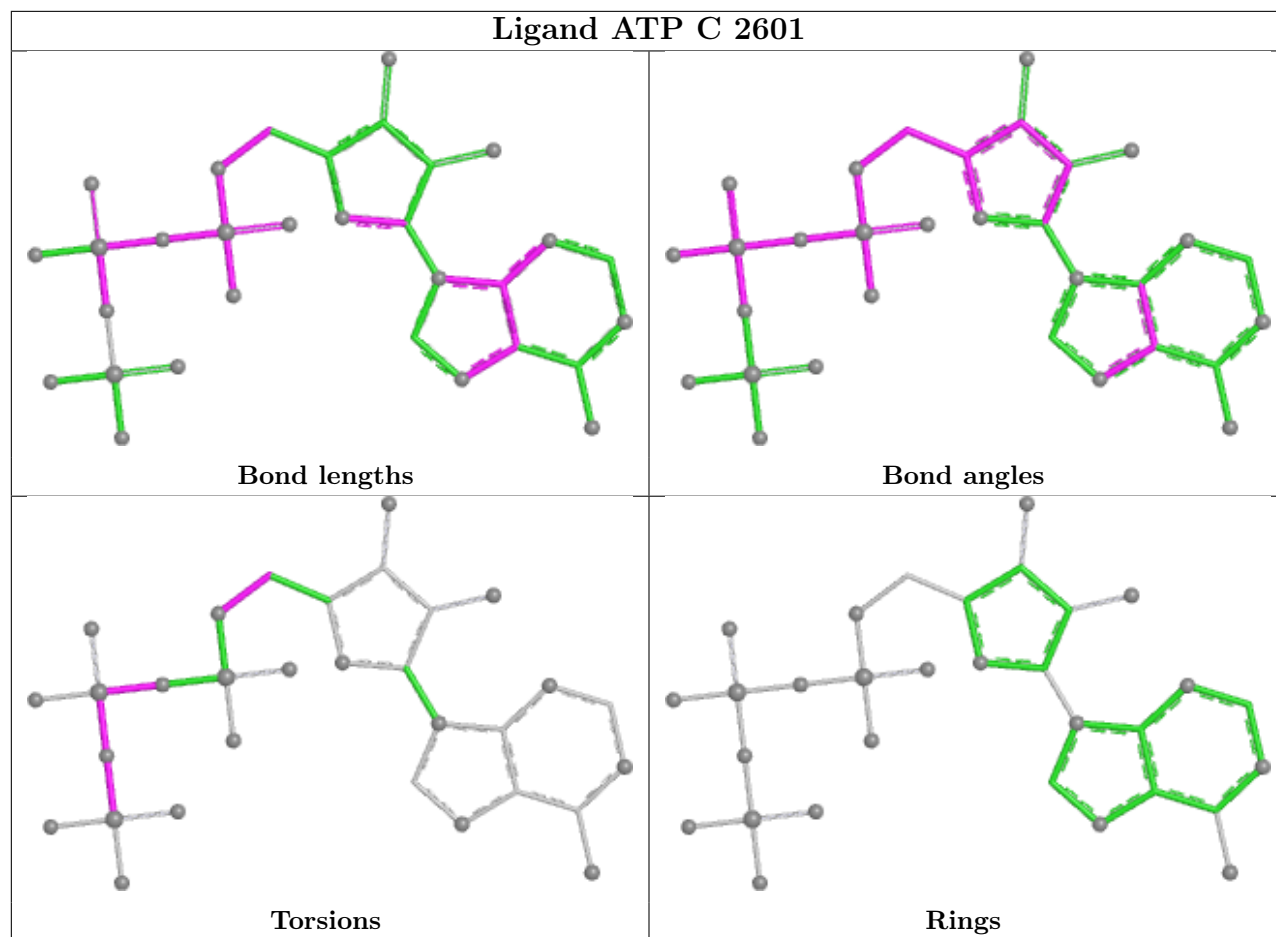


Ligand ADP D 3600



Ligand ATP A 601





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	242/243 (99%)	-1.55	0 100 100	20, 57, 130, 176	0
1	B	242/243 (99%)	-1.43	0 100 100	26, 84, 144, 170	0
1	C	242/243 (99%)	-1.54	0 100 100	17, 57, 126, 176	0
1	D	241/243 (99%)	-1.42	0 100 100	24, 86, 145, 153	0
All	All	967/972 (99%)	-1.48	0 100 100	17, 67, 145, 176	0

There are no RSRZ outliers to report.

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.

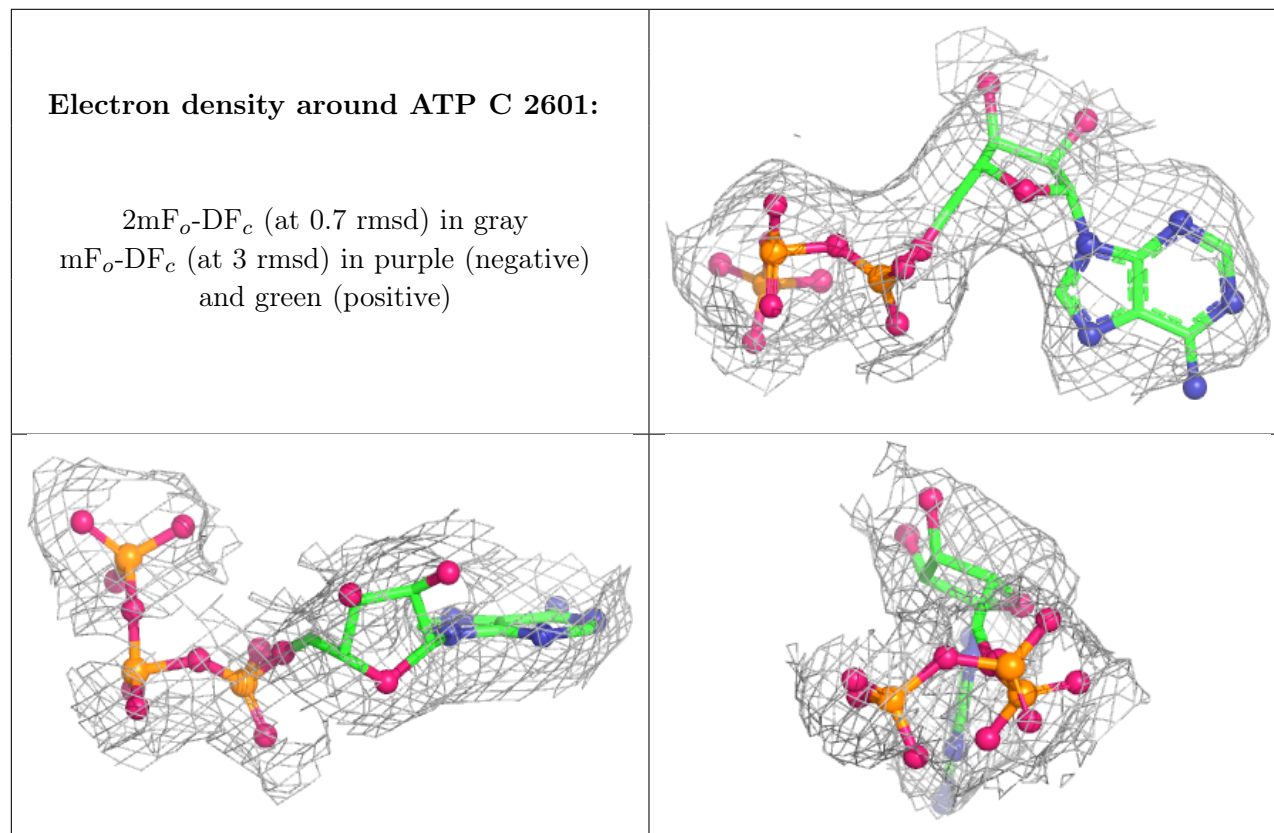
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	C	1601	1/1	0.96	0.07	76,76,76,76	0
4	MG	D	3601	1/1	0.98	0.04	36,36,36,36	0
2	ATP	C	2601	31/31	0.99	0.02	37,52,89,95	0
3	ADP	D	3600	27/27	1.00	0.03	17,37,50,52	0

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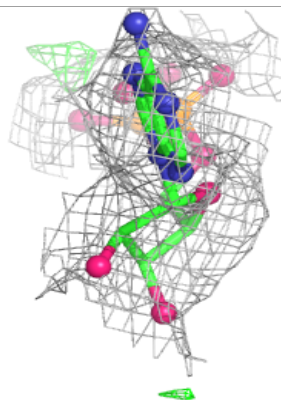
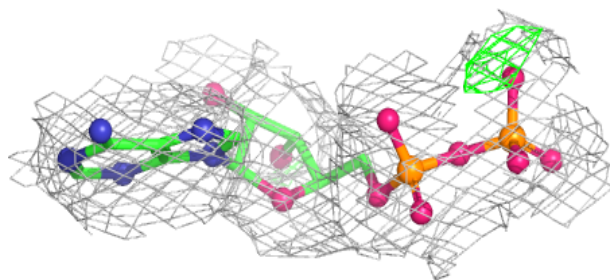
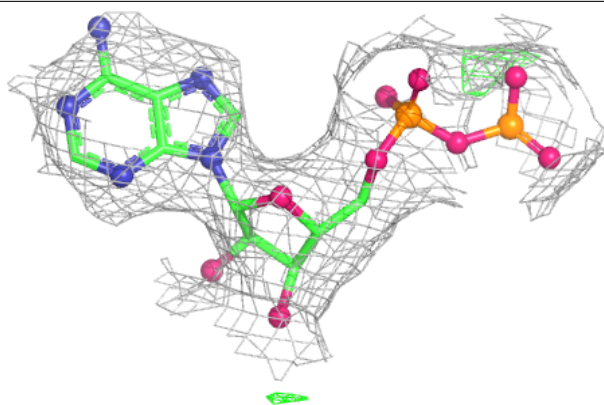
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	A	601	31/31	1.00	0.03	49,57,97,99	0
3	ADP	B	1600	27/27	1.00	0.02	19,42,53,54	0

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.

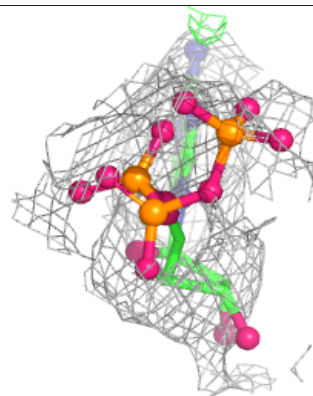
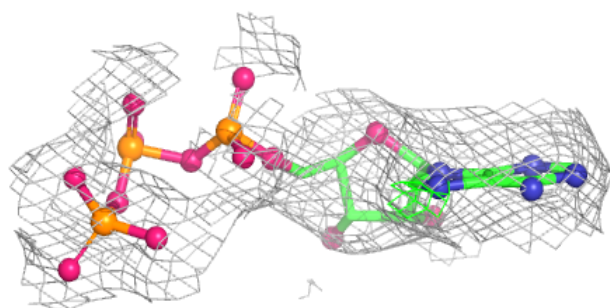
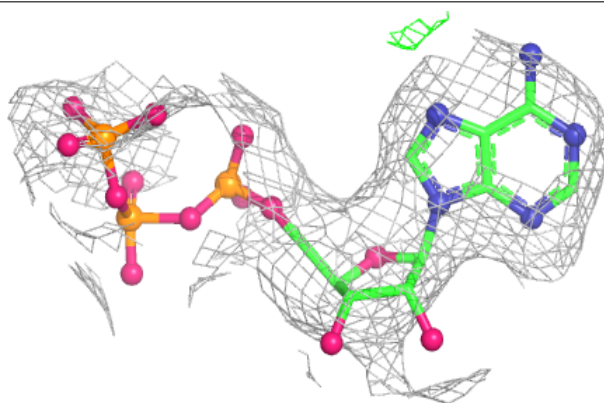


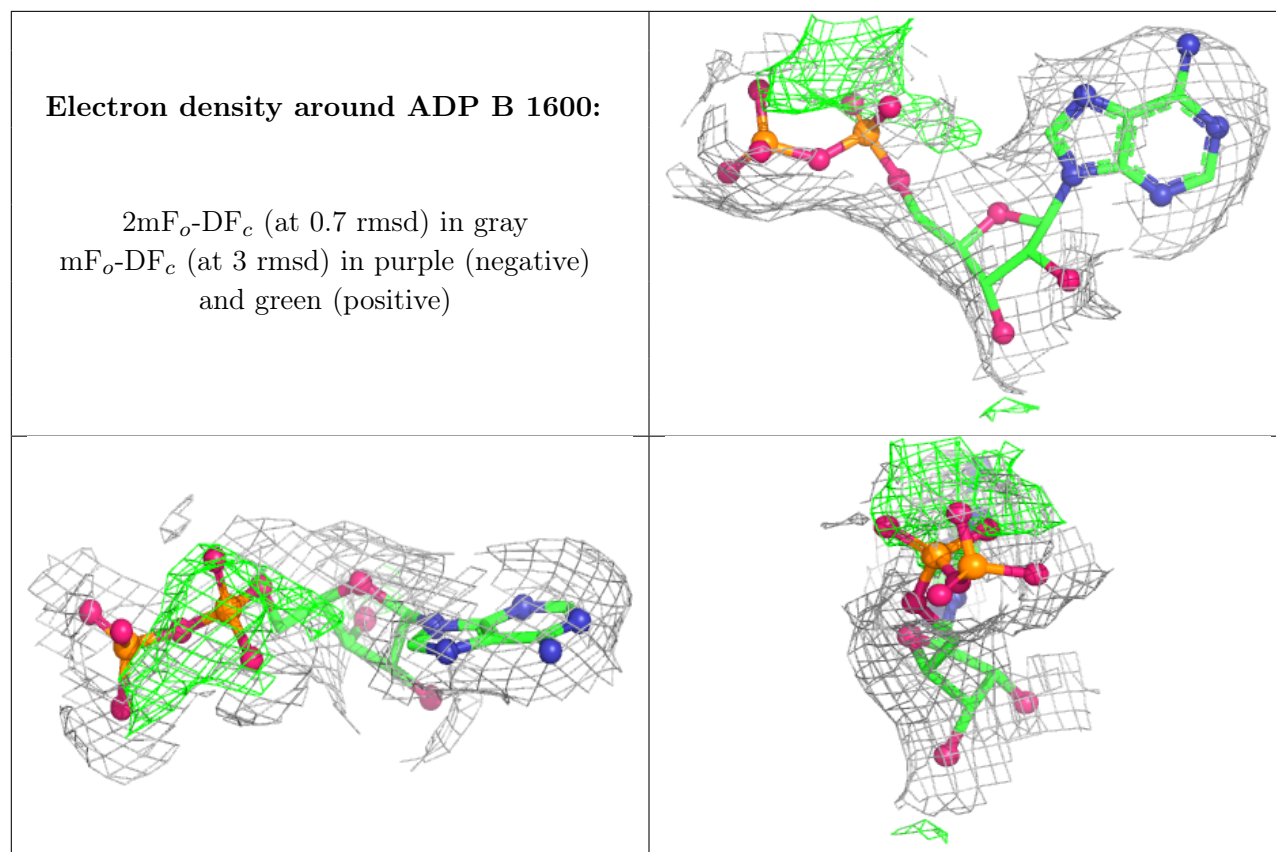
Electron density around ADP D 3600:

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

**Electron density around ATP 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.