



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:47 AM UTC

PDB ID : 1E8H / pdb_00001e8h
Title : STRUCTURE OF THE H61T MUTANT OF THE FLAVOENZYME
VANILLYL-ALCOHOL OXIDASE IN THE APO FORM COMPLEXED BY
ADP
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Deposited on : 2000-09-20
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

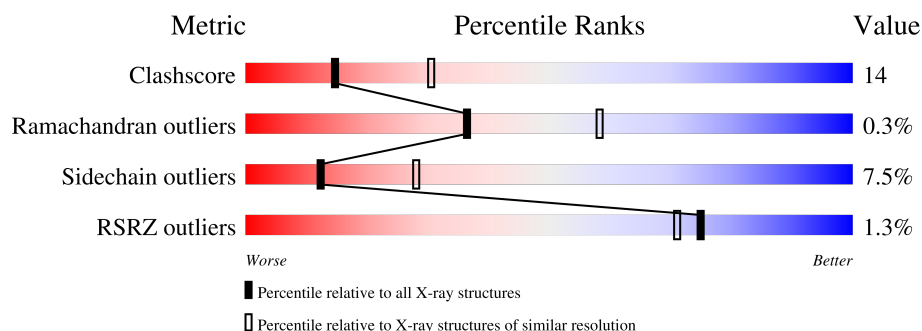
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	560	 55% 31% 9% . .
1	B	560	 56% 31% 9% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8765 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 VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	125	0	0
			4311	2768	737	782	24			
1	B	545	Total	C	N	O	S	125	0	0
			4311	2768	737	782	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	HIS	engineered mutation	UNP P56216
B	61	THR	HIS	engineered mutation	UNP P56216

- 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	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

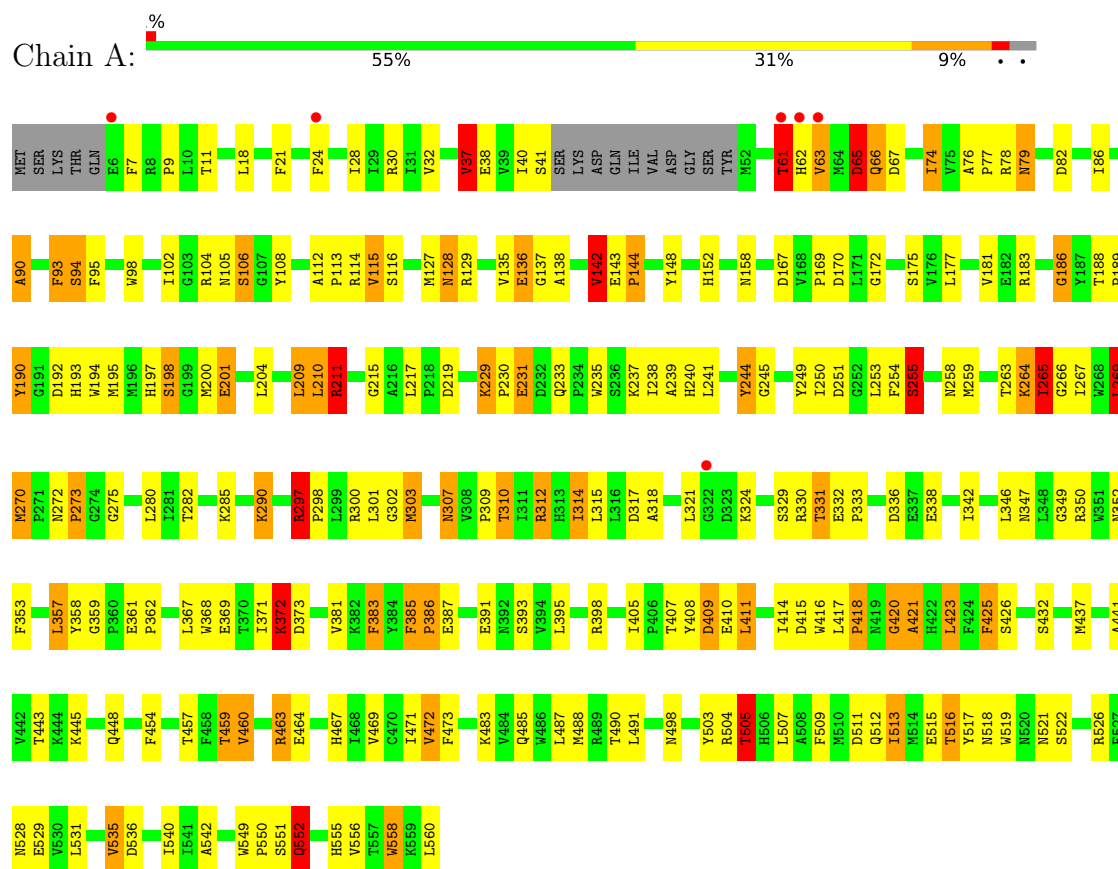
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	43	Total	O	0	0
			43	43		

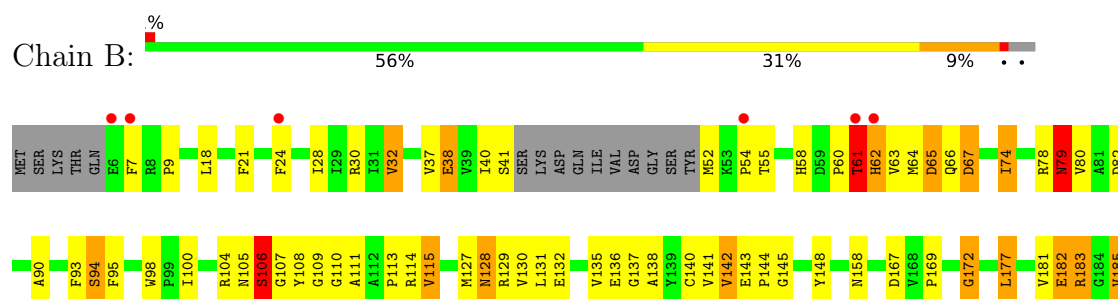
3 Residue-property plots

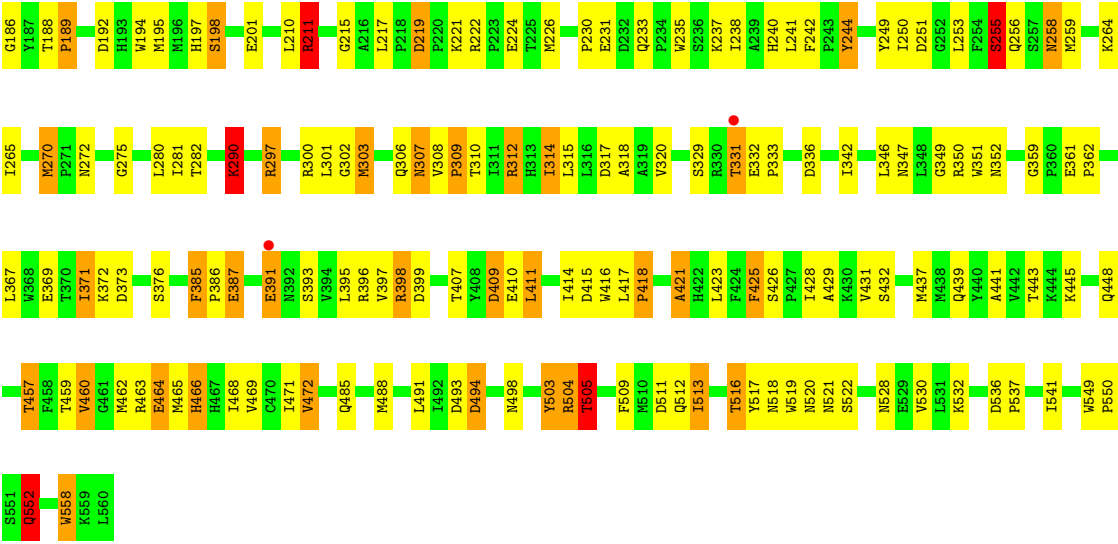
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: VANILLYL-ALCOHOL OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	130.34Å 130.34Å 134.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.60) 99.2 (20.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.303 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.000 for -l,-k,-h 0.012 for -h,-l,-k 0.000 for -h,l,k 0.025 for -h,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8765	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	3/4428 (0.1%)	2.06	170/6018 (2.8%)
1	B	0.77	4/4428 (0.1%)	2.00	136/6018 (2.3%)
All	All	0.78	7/8856 (0.1%)	2.03	306/12036 (2.5%)

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	A	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	LYS	CG-CD	-8.10	1.28	1.52
1	A	67	ASP	CA-CB	-7.65	1.40	1.53
1	B	67	ASP	CA-CB	-7.51	1.40	1.53
1	B	221	LYS	CG-CD	-7.37	1.30	1.52
1	A	229	LYS	CG-CD	-5.96	1.34	1.52
1	B	66	GLN	CA-CB	5.48	1.62	1.53
1	A	483	LYS	CG-CD	-5.10	1.37	1.52

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CD-NE-CZ	27.78	163.29	124.40
1	A	211	ARG	CD-NE-CZ	25.40	159.96	124.40
1	A	7	PHE	N-CA-C	17.75	133.52	111.69
1	B	7	PHE	N-CA-C	16.87	135.90	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	485	GLN	OE1-CD-NE2	-14.26	108.34	122.60
1	A	485	GLN	OE1-CD-NE2	-13.68	108.92	122.60
1	A	24	PHE	CA-CB-CG	13.20	127.00	113.80
1	B	24	PHE	CA-CB-CG	12.91	126.71	113.80
1	B	211	ARG	CA-CB-CG	12.69	139.47	114.10
1	A	211	ARG	CA-CB-CG	12.23	138.56	114.10
1	B	104	ARG	CD-NE-CZ	12.17	141.44	124.40
1	B	536	ASP	CA-CB-CG	11.89	124.50	112.60
1	B	127	MET	CA-C-N	11.55	140.63	122.26
1	B	127	MET	C-N-CA	11.55	140.63	122.26
1	A	467	HIS	O-C-N	-11.52	109.53	122.55
1	A	65	ASP	CA-CB-CG	11.42	124.02	112.60
1	A	127	MET	CA-C-N	11.11	141.49	122.26
1	A	127	MET	C-N-CA	11.11	141.49	122.26
1	B	221	LYS	CB-CG-CD	11.10	136.83	111.30
1	B	183	ARG	CD-NE-CZ	10.97	139.76	124.40
1	B	128	ASN	CA-CB-CG	10.54	123.14	112.60
1	B	372	LYS	CG-CD-CE	10.41	135.25	111.30
1	A	536	ASP	CA-CB-CG	10.34	122.94	112.60
1	A	312	ARG	NE-CZ-NH2	-10.29	109.94	119.20
1	B	307	ASN	CA-C-N	-10.20	115.66	122.60
1	B	307	ASN	C-N-CA	-10.20	115.66	122.60
1	A	190	TYR	CA-C-N	9.99	131.07	119.98
1	A	190	TYR	C-N-CA	9.99	131.07	119.98
1	B	448	GLN	OE1-CD-NE2	-9.86	112.74	122.60
1	A	448	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	B	66	GLN	OE1-CD-NE2	-9.67	112.93	122.60
1	A	66	GLN	OE1-CD-NE2	-9.65	112.95	122.60
1	A	128	ASN	CA-CB-CG	9.54	122.14	112.60
1	B	65	ASP	CA-CB-CG	9.44	122.04	112.60
1	B	182	GLU	CA-C-O	8.97	130.87	119.12
1	A	235	TRP	CA-C-O	-8.94	111.06	121.16
1	B	219	ASP	CA-CB-CG	8.88	121.48	112.60
1	A	536	ASP	CA-C-N	8.83	129.71	119.47
1	A	536	ASP	C-N-CA	8.83	129.71	119.47
1	B	300	ARG	CD-NE-CZ	8.64	136.49	124.40
1	B	106	SER	CA-C-N	-8.51	113.55	123.08
1	B	106	SER	C-N-CA	-8.51	113.55	123.08
1	A	37	VAL	CA-C-O	-8.43	110.25	120.78
1	A	372	LYS	CG-CD-CE	8.37	130.54	111.30
1	B	558	TRP	N-CA-C	8.19	123.40	113.41
1	B	532	LYS	CA-C-O	-8.10	111.83	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	ILE	N-CA-C	8.07	118.83	107.37
1	A	104	ARG	CD-NE-CZ	8.06	135.69	124.40
1	B	128	ASN	CB-CA-C	-7.96	96.18	109.55
1	B	504	ARG	CD-NE-CZ	7.88	135.43	124.40
1	B	466	HIS	CA-C-O	-7.75	112.28	120.58
1	B	107	GLY	N-CA-C	-7.73	105.28	114.48
1	A	421	ALA	N-CA-C	-7.72	97.59	109.24
1	A	37	VAL	O-C-N	-7.71	112.93	122.57
1	A	405	ILE	CA-C-O	7.71	123.70	119.15
1	A	61	THR	N-CA-C	-7.64	101.02	110.65
1	B	61	THR	CB-CA-C	7.64	122.21	111.74
1	B	528	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	B	464	GLU	CB-CG-CD	7.59	125.50	112.60
1	B	242	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	513	ILE	CA-C-O	-7.58	113.06	120.95
1	A	542	ALA	N-CA-CB	-7.51	103.33	111.66
1	A	61	THR	CB-CA-C	7.50	122.02	111.74
1	A	142	VAL	N-CA-CB	-7.47	97.95	111.92
1	A	129	ARG	N-CA-C	7.43	121.94	110.20
1	A	128	ASN	CB-CA-C	-7.39	96.78	109.65
1	B	129	ARG	N-CA-C	7.33	121.41	109.76
1	A	255	SER	N-CA-CB	7.32	122.59	110.52
1	A	555	HIS	CA-C-N	7.32	129.78	120.56
1	A	555	HIS	C-N-CA	7.32	129.78	120.56
1	A	558	TRP	N-CA-C	7.27	122.45	113.50
1	A	128	ASN	N-CA-C	7.25	122.29	113.38
1	A	560	LEU	CA-C-O	-7.24	108.50	120.80
1	A	464	GLU	CB-CG-CD	7.21	124.86	112.60
1	A	312	ARG	NE-CZ-NH1	7.21	128.71	121.50
1	A	383	PHE	N-CA-CB	-7.20	98.68	110.42
1	A	254	PHE	CA-C-O	-7.19	111.15	119.56
1	B	135	VAL	N-CA-C	7.16	117.26	110.53
1	A	128	ASN	N-CA-CB	-7.14	99.90	110.53
1	B	61	THR	N-CA-C	-7.13	101.67	110.65
1	B	312	ARG	NE-CZ-NH2	-7.05	112.86	119.20
1	A	556	VAL	N-CA-CB	7.04	118.79	110.55
1	A	186	GLY	O-C-N	-7.01	117.50	123.59
1	B	460	VAL	N-CA-C	6.99	118.54	107.98
1	A	135	VAL	N-CA-C	6.97	117.08	110.53
1	A	536	ASP	O-C-N	-6.97	115.14	121.34
1	A	426	SER	N-CA-C	6.90	121.53	108.97
1	A	512	GLN	OE1-CD-NE2	6.85	129.45	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ILE	CA-C-O	-6.80	112.97	120.72
1	A	66	GLN	CG-CD-NE2	6.77	126.56	116.40
1	B	331	THR	N-CA-C	-6.75	105.33	113.97
1	B	128	ASN	N-CA-CB	-6.71	100.79	110.65
1	A	460	VAL	N-CA-C	6.70	117.39	107.15
1	A	106	SER	CA-C-N	-6.69	114.04	123.08
1	A	106	SER	C-N-CA	-6.69	114.04	123.08
1	B	169	PRO	CB-CA-C	6.68	121.31	111.22
1	B	255	SER	N-CA-CB	6.68	121.54	110.52
1	A	74	ILE	CA-C-O	-6.66	113.42	120.48
1	B	448	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	448	GLN	CG-CD-NE2	6.65	126.37	116.40
1	B	66	GLN	CG-CD-NE2	6.58	126.26	116.40
1	B	282	THR	CA-C-O	6.57	127.59	120.43
1	B	244	TYR	CA-C-O	-6.53	111.21	119.31
1	A	300	ARG	CD-NE-CZ	6.51	133.52	124.40
1	A	267	ILE	O-C-N	-6.51	116.15	123.18
1	B	142	VAL	N-CA-CB	-6.51	99.75	111.92
1	B	221	LYS	CG-CD-CE	6.50	126.26	111.30
1	B	185	VAL	CB-CA-C	-6.46	100.56	110.50
1	B	128	ASN	N-CA-C	6.45	122.11	113.72
1	A	108	TYR	N-CA-C	-6.44	103.71	113.89
1	B	421	ALA	N-CA-C	-6.42	99.55	109.24
1	B	552	GLN	CA-CB-CG	6.35	126.79	114.10
1	B	308	VAL	N-CA-C	-6.34	101.79	107.56
1	A	467	HIS	N-CA-C	6.33	119.70	108.24
1	A	65	ASP	CA-C-N	6.32	129.81	120.90
1	A	65	ASP	C-N-CA	6.32	129.81	120.90
1	B	127	MET	CA-C-O	6.32	129.63	122.37
1	B	409	ASP	N-CA-C	6.32	118.72	111.02
1	A	420	GLY	CA-C-O	6.29	128.69	121.90
1	A	509	PHE	CA-C-O	6.29	126.60	119.18
1	B	385	PHE	N-CA-CB	6.28	116.87	109.72
1	B	235	TRP	CA-C-O	-6.27	113.97	121.56
1	A	142	VAL	N-CA-C	6.27	118.97	108.81
1	B	290	LYS	CB-CG-CD	6.26	125.70	111.30
1	B	512	GLN	OE1-CD-NE2	6.25	128.85	122.60
1	A	487	LEU	CA-C-O	6.24	127.94	121.07
1	A	219	ASP	CA-C-N	6.22	126.24	119.89
1	A	219	ASP	C-N-CA	6.22	126.24	119.89
1	A	498	ASN	CA-CB-CG	-6.22	106.38	112.60
1	B	128	ASN	CB-CG-ND2	6.22	125.72	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ARG	CA-C-O	6.19	127.17	120.55
1	B	494	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	65	ASP	N-CA-CB	-6.15	101.58	110.87
1	B	509	PHE	CA-CB-CG	-6.14	107.66	113.80
1	B	108	TYR	N-CA-C	-6.11	104.23	113.89
1	B	183	ARG	O-C-N	-6.08	114.26	122.41
1	A	66	GLN	CA-C-O	6.08	127.84	121.15
1	B	66	GLN	CA-C-O	6.06	127.82	121.15
1	B	158	ASN	CA-CB-CG	6.06	118.66	112.60
1	B	142	VAL	N-CA-C	6.05	118.61	108.81
1	A	229	LYS	CB-CG-CD	6.04	125.20	111.30
1	A	211	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	A	505	THR	CB-CA-C	-6.04	97.58	111.95
1	A	285	LYS	N-CA-C	6.03	119.65	109.76
1	B	513	ILE	CA-C-O	-6.03	114.68	120.95
1	B	32	VAL	N-CA-C	6.03	118.80	112.83
1	B	398	ARG	CA-C-O	-6.02	111.97	119.38
1	B	226	MET	CA-CB-CG	6.02	126.14	114.10
1	A	211	ARG	N-CA-CB	6.01	121.19	110.80
1	A	529	GLU	CA-C-N	5.98	128.10	120.56
1	A	529	GLU	C-N-CA	5.98	128.10	120.56
1	A	551	SER	N-CA-C	5.98	118.58	111.71
1	A	556	VAL	O-C-N	5.97	127.76	121.91
1	A	358	TYR	CA-C-O	-5.97	114.42	121.16
1	A	201	GLU	CA-C-O	5.96	126.92	120.43
1	A	556	VAL	N-CA-C	-5.95	104.71	110.42
1	A	266	GLY	CA-C-O	-5.92	115.75	120.91
1	A	471	ILE	CA-C-N	-5.91	115.47	123.10
1	A	471	ILE	C-N-CA	-5.91	115.47	123.10
1	B	250	ILE	O-C-N	5.91	128.57	122.07
1	B	172	GLY	N-CA-C	5.89	123.03	115.32
1	B	185	VAL	N-CA-C	5.89	117.23	108.46
1	A	244	TYR	CA-C-O	-5.88	112.01	119.31
1	A	105	ASN	N-CA-C	5.86	118.41	109.62
1	A	258	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	290	LYS	CB-CG-CD	5.85	124.75	111.30
1	A	386	PRO	CA-C-N	5.85	128.92	120.38
1	A	386	PRO	C-N-CA	5.85	128.92	120.38
1	A	244	TYR	N-CA-C	5.83	120.12	112.89
1	B	425	PHE	N-CA-C	-5.82	99.25	108.73
1	A	259	MET	CA-C-O	-5.81	112.23	119.38
1	B	93	PHE	CA-C-O	-5.81	112.27	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	THR	CB-CA-C	-5.80	98.14	111.95
1	A	193	HIS	N-CA-C	5.80	118.07	111.11
1	A	504	ARG	CD-NE-CZ	5.80	132.52	124.40
1	A	409	ASP	N-CA-C	5.79	118.08	111.02
1	A	270	MET	CA-C-O	5.78	123.60	119.32
1	A	143	GLU	CA-C-N	5.78	125.91	119.32
1	A	143	GLU	C-N-CA	5.78	125.91	119.32
1	A	515	GLU	CA-C-N	5.77	128.58	120.28
1	A	515	GLU	C-N-CA	5.77	128.58	120.28
1	A	310	THR	CA-C-N	-5.74	115.29	123.10
1	A	310	THR	C-N-CA	-5.74	115.29	123.10
1	B	306	GLN	N-CA-C	5.74	118.75	111.69
1	B	308	VAL	N-CA-CB	5.71	117.54	111.20
1	B	145	GLY	N-CA-C	5.71	121.07	114.16
1	A	490	THR	N-CA-C	-5.69	104.45	111.40
1	B	198	SER	CA-C-O	-5.68	113.33	119.98
1	A	90	ALA	CA-C-O	-5.67	114.40	120.42
1	A	485	GLN	CG-CD-NE2	5.67	124.91	116.40
1	A	239	ALA	CA-C-O	5.67	127.27	120.92
1	A	158	ASN	CA-CB-CG	5.66	118.26	112.60
1	B	80	VAL	CA-C-O	-5.65	115.08	120.95
1	B	256	GLN	OE1-CD-NE2	-5.64	116.95	122.60
1	A	249	TYR	CA-C-N	5.62	130.22	121.35
1	A	249	TYR	C-N-CA	5.62	130.22	121.35
1	B	351	TRP	CA-C-O	-5.61	114.90	121.46
1	B	520	ASN	O-C-N	-5.60	115.57	122.57
1	A	385	PHE	N-CA-C	-5.60	103.07	110.40
1	A	357	LEU	N-CA-CB	-5.59	101.32	110.43
1	A	542	ALA	CB-CA-C	-5.59	107.23	111.20
1	A	385	PHE	N-CA-CB	5.58	117.81	109.88
1	B	471	ILE	CA-C-N	-5.58	115.91	123.10
1	B	471	ILE	C-N-CA	-5.58	115.91	123.10
1	A	331	THR	N-CA-C	-5.56	106.86	113.97
1	B	65	ASP	CA-C-N	5.55	128.73	120.90
1	B	65	ASP	C-N-CA	5.55	128.73	120.90
1	A	136	GLU	CA-CB-CG	5.54	125.18	114.10
1	A	193	HIS	CA-CB-CG	-5.53	108.27	113.80
1	A	192	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	129	ARG	CA-C-O	5.51	127.33	121.05
1	A	215	GLY	N-CA-C	-5.50	108.62	114.67
1	A	230	PRO	CA-C-O	5.50	128.74	120.05
1	A	258	ASN	CA-C-O	5.50	126.60	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	B	183	ARG	N-CA-C	5.48	119.14	111.74
1	B	272	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	B	37	VAL	CA-C-O	-5.45	114.79	120.51
1	A	542	ALA	O-C-N	-5.44	119.03	121.53
1	A	459	THR	N-CA-C	-5.39	100.40	109.07
1	B	62	HIS	CA-C-O	-5.39	115.09	120.96
1	A	526	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	115	VAL	N-CA-CB	5.37	118.55	111.25
1	B	426	SER	N-CA-CB	-5.36	103.33	111.21
1	A	169	PRO	CB-CA-C	5.36	118.68	110.75
1	A	408	TYR	CA-C-N	5.35	128.23	120.79
1	A	408	TYR	C-N-CA	5.35	128.23	120.79
1	A	211	ARG	NE-CZ-NH2	-5.35	114.39	119.20
1	B	130	VAL	N-CA-C	-5.35	100.95	108.12
1	A	555	HIS	CA-CB-CG	5.34	119.14	113.80
1	B	38	GLU	CA-C-N	5.34	129.25	122.37
1	B	38	GLU	C-N-CA	5.34	129.25	122.37
1	B	270	MET	CA-C-O	5.33	123.56	119.46
1	A	198	SER	O-C-N	5.32	129.66	122.59
1	A	269	LEU	O-C-N	-5.31	116.97	123.19
1	A	421	ALA	CA-C-O	-5.30	115.41	121.40
1	B	426	SER	N-CA-C	5.30	119.51	108.39
1	A	528	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	93	PHE	CA-C-N	-5.29	114.99	122.34
1	A	93	PHE	C-N-CA	-5.29	114.99	122.34
1	B	498	ASN	CA-CB-CG	-5.28	107.32	112.60
1	B	372	LYS	CB-CG-CD	5.28	123.44	111.30
1	A	552	GLN	CA-C-N	5.27	131.08	123.13
1	A	552	GLN	C-N-CA	5.27	131.08	123.13
1	B	79	ASN	N-CA-C	5.26	115.18	108.24
1	B	397	VAL	CB-CA-C	-5.26	105.24	111.97
1	A	264	LYS	CA-C-N	-5.25	114.92	121.96
1	A	264	LYS	C-N-CA	-5.25	114.92	121.96
1	A	297	ARG	CA-C-N	5.25	124.88	119.05
1	A	297	ARG	C-N-CA	5.25	124.88	119.05
1	A	265	ILE	CA-C-N	-5.25	117.21	122.20
1	A	265	ILE	C-N-CA	-5.25	117.21	122.20
1	A	86	ILE	O-C-N	-5.25	116.57	121.87
1	A	505	THR	O-C-N	5.25	129.06	122.92
1	B	255	SER	CB-CA-C	-5.23	100.69	109.48
1	A	459	THR	CB-CA-C	5.22	118.75	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	B	237	LYS	N-CA-C	5.21	117.63	111.33
1	A	209	LEU	CA-C-O	-5.21	115.11	121.05
1	B	105	ASN	N-CA-C	5.20	117.42	109.62
1	A	170	ASP	CA-C-O	-5.20	114.38	120.20
1	B	182	GLU	N-CA-C	5.20	119.49	113.20
1	B	258	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	A	423	LEU	CA-C-O	-5.19	115.04	121.06
1	B	457	THR	CB-CA-C	-5.19	98.66	110.07
1	A	63	VAL	N-CA-CB	5.17	119.77	111.23
1	A	210	LEU	CA-C-O	-5.17	114.18	120.54
1	A	204	LEU	N-CA-C	5.17	116.77	110.41
1	A	169	PRO	CA-C-O	-5.17	115.33	122.15
1	A	250	ILE	CB-CG1-CD1	-5.15	102.98	113.80
1	B	215	GLY	N-CA-C	-5.15	107.93	114.16
1	B	78	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	B	537	PRO	CA-C-O	-5.14	111.83	119.18
1	B	249	TYR	CB-CA-C	5.14	119.95	111.31
1	A	237	LYS	N-CA-C	5.13	116.87	111.28
1	B	309	PRO	CA-C-O	-5.13	115.32	121.48
1	A	425	PHE	N-CA-C	-5.11	100.40	108.73
1	B	297	ARG	CA-C-N	5.11	124.72	119.05
1	B	297	ARG	C-N-CA	5.11	124.72	119.05
1	A	321	LEU	N-CA-C	5.10	117.74	111.82
1	B	468	ILE	CB-CA-C	-5.09	106.40	111.80
1	B	259	MET	CA-C-O	-5.08	112.61	119.11
1	A	307	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	64	MET	CA-C-N	-5.08	113.24	123.09
1	B	64	MET	C-N-CA	-5.08	113.24	123.09
1	B	169	PRO	N-CA-C	-5.07	104.12	111.22
1	B	371	ILE	CA-C-N	5.06	128.41	120.82
1	B	371	ILE	C-N-CA	5.06	128.41	120.82
1	A	393	SER	CA-C-N	5.06	127.39	120.46
1	A	393	SER	C-N-CA	5.06	127.39	120.46
1	B	320	VAL	N-CA-C	-5.05	105.58	110.42
1	B	192	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	209	LEU	O-C-N	5.04	128.96	123.01
1	A	273	PRO	CB-CA-C	5.04	116.77	110.27
1	B	536	ASP	CA-C-N	5.04	124.70	119.56
1	B	536	ASP	C-N-CA	5.04	124.70	119.56
1	A	552	GLN	CA-CB-CG	5.04	124.17	114.10
1	B	189	PRO	O-C-N	-5.03	115.50	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	PRO	CA-C-N	5.02	129.73	120.79
1	A	144	PRO	C-N-CA	5.02	129.73	120.79
1	B	312	ARG	CD-NE-CZ	5.02	131.43	124.40
1	B	393	SER	CA-C-O	5.02	126.87	121.55
1	B	61	THR	N-CA-CB	-5.01	104.58	110.35
1	A	200	MET	CA-CB-CG	5.01	124.13	114.10
1	A	535	VAL	CA-C-O	-5.01	113.52	119.58
1	B	530	VAL	CA-C-O	-5.00	115.87	121.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	LEU	Mainchain
1	A	37	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	4311	0	4260	125	3
1	B	4311	0	4260	125	2
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	46	0	0	5	0
3	B	43	0	0	2	0
All	All	8765	0	8544	231	4

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 14.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG11	1:B:423:LEU:HD11	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG11	1:A:423:LEU:HD11	1.43	1.01
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.51	0.92
1:B:40:ILE:HD11	1:B:74:ILE:HD11	1.54	0.89
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.54	0.88
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.94	0.82
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.62	0.81
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.64	0.79
1:B:181:VAL:O	1:B:255:SER:HB3	1.85	0.77
1:A:552:GLN:NE2	1:A:552:GLN:H	1.83	0.76
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.00	0.76
1:B:349:GLY:H	1:B:352:ASN:HD21	1.34	0.76
1:B:552:GLN:NE2	1:B:552:GLN:H	1.86	0.73
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.70	0.72
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.72	0.71
1:B:79:ASN:ND2	1:B:82:ASP:H	1.90	0.70
1:A:40:ILE:HD11	1:A:74:ILE:HD11	1.72	0.70
1:A:79:ASN:HD22	1:A:82:ASP:H	1.42	0.68
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.58	0.67
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.74	0.67
1:A:181:VAL:O	1:A:255:SER:HB3	1.95	0.66
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.78	0.65
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.26	0.65
1:A:79:ASN:ND2	1:A:82:ASP:H	1.94	0.65
1:A:315:LEU:HA	1:A:318:ALA:HB3	1.79	0.65
1:B:275:GLY:HA3	1:B:359:GLY:O	1.97	0.65
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.78	0.65
1:B:167:ASP:OD1	1:B:186:GLY:HA3	1.95	0.65
1:B:79:ASN:HD22	1:B:82:ASP:H	1.45	0.64
1:A:411:LEU:O	1:A:414:ILE:HG12	1.98	0.63
1:B:407:THR:HB	1:B:409:ASP:OD1	1.98	0.63
1:B:183:ARG:HH11	1:B:255:SER:HB2	1.64	0.63
1:A:349:GLY:H	1:A:352:ASN:HD21	1.44	0.62
1:A:369:GLU:O	1:A:373:ASP:HB2	1.99	0.62
1:B:552:GLN:H	1:B:552:GLN:HE21	1.47	0.62
1:A:552:GLN:H	1:A:552:GLN:HE21	1.48	0.62
1:B:280:LEU:HB3	1:B:395:LEU:HD22	1.82	0.62
1:A:275:GLY:HA3	1:A:359:GLY:O	1.99	0.61
1:B:315:LEU:HA	1:B:318:ALA:HB3	1.83	0.61
1:B:513:ILE:O	1:B:516:THR:HB	2.01	0.61
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.31	0.60
1:A:183:ARG:NH1	1:A:255:SER:HB2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLU:O	1:B:373:ASP:HB2	2.02	0.60
1:B:346:LEU:O	1:B:347:ASN:HB2	2.02	0.60
1:B:310:THR:HG22	1:B:459:THR:HG22	1.84	0.60
1:A:346:LEU:O	1:A:347:ASN:HB2	2.02	0.60
1:B:201:GLU:OE2	1:B:264:LYS:NZ	2.34	0.59
1:A:136:GLU:HG2	3:A:2005:HOH:O	2.02	0.59
1:A:518:ASN:O	1:A:519:TRP:C	2.44	0.59
1:B:194:TRP:O	1:B:197:HIS:HD2	1.84	0.59
1:A:65:ASP:OD1	1:A:66:GLN:N	2.36	0.59
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.02	0.59
1:A:381:VAL:HG12	3:A:2026:HOH:O	2.02	0.59
1:B:411:LEU:O	1:B:414:ILE:HG12	2.03	0.58
1:A:513:ILE:O	1:A:516:THR:HB	2.03	0.58
1:A:194:TRP:O	1:A:197:HIS:HD2	1.86	0.58
1:B:521:ASN:O	1:B:522:SER:HB2	2.03	0.57
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.87	0.57
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.40	0.57
1:A:521:ASN:O	1:A:522:SER:HB2	2.04	0.57
1:B:148:TYR:HB2	1:B:172:GLY:O	2.05	0.57
1:B:416:TRP:HB3	1:B:472:VAL:HG21	1.86	0.57
1:A:290:LYS:HB2	1:A:437:MET:HG3	1.88	0.56
1:A:188:THR:HB	1:A:189:PRO:CD	2.36	0.56
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.41	0.56
1:A:373:ASP:HB3	3:A:2024:HOH:O	2.06	0.56
1:A:253:LEU:CD2	1:B:253:LEU:HD21	2.35	0.55
1:B:307:ASN:O	1:B:309:PRO:HD3	2.07	0.55
1:B:425:PHE:HA	1:B:488:MET:HE1	1.89	0.55
1:B:115:VAL:HG13	3:B:2040:HOH:O	2.05	0.55
1:A:244:TYR:OH	1:B:195:MET:HE2	2.07	0.55
1:A:37:VAL:HG12	1:A:37:VAL:O	2.06	0.55
1:A:269:LEU:O	1:B:463:ARG:NH2	2.39	0.55
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.88	0.54
1:B:518:ASN:O	1:B:519:TRP:C	2.48	0.54
1:A:443:THR:HG21	1:A:469:VAL:CG2	2.37	0.54
1:A:420:GLY:HA2	1:A:473:PHE:O	2.08	0.54
1:A:253:LEU:HD21	1:B:253:LEU:CD2	2.36	0.54
1:A:183:ARG:HH11	1:A:255:SER:HB2	1.72	0.54
1:A:241:LEU:HB3	1:B:463:ARG:O	2.08	0.54
1:A:195:MET:HE2	1:B:244:TYR:OH	2.08	0.54
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.89	0.53
1:B:183:ARG:NH1	1:B:255:SER:HB2	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ARG:NH2	1:A:410:GLU:OE1	2.41	0.53
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.89	0.53
1:B:201:GLU:HB3	1:B:264:LYS:HB2	1.89	0.53
1:A:148:TYR:HB2	1:A:172:GLY:O	2.09	0.53
1:A:189:PRO:HG2	1:A:270:MET:CE	2.32	0.53
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.90	0.53
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.44	0.53
1:A:152:HIS:HD2	3:A:2029:HOH:O	1.91	0.52
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.91	0.52
1:B:290:LYS:HB2	1:B:437:MET:HG3	1.90	0.52
1:A:463:ARG:O	1:B:241:LEU:HB3	2.09	0.52
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.45	0.51
1:B:189:PRO:HG2	1:B:270:MET:CE	2.32	0.51
1:A:61:THR:OG1	1:A:421:ALA:HB1	2.10	0.51
1:A:443:THR:HA	1:A:491:LEU:HD21	1.93	0.51
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.41	0.51
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.92	0.51
1:A:415:ASP:O	1:A:416:TRP:C	2.52	0.51
1:A:531:LEU:O	1:A:535:VAL:HG22	2.11	0.51
1:B:185:VAL:HG12	1:B:186:GLY:N	2.24	0.51
1:A:188:THR:CB	1:A:189:PRO:CD	2.90	0.50
1:A:505:THR:HG23	3:A:2031:HOH:O	2.11	0.50
1:B:516:THR:HG21	3:B:2032:HOH:O	2.11	0.50
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.41	0.50
1:B:290:LYS:HB2	1:B:437:MET:CG	2.41	0.50
1:A:11:THR:HG21	1:A:116:SER:HB3	1.95	0.49
1:B:312:ARG:HD3	1:B:317:ASP:OD1	2.12	0.49
1:B:79:ASN:HD22	1:B:79:ASN:C	2.20	0.49
1:A:38:GLU:HB3	1:A:74:ILE:HD13	1.95	0.49
1:A:290:LYS:HB2	1:A:437:MET:CG	2.42	0.49
1:A:114:ARG:NH2	1:A:511:ASP:OD2	2.46	0.49
1:B:219:ASP:OD2	1:B:222:ARG:NH1	2.46	0.48
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.95	0.48
1:B:443:THR:HA	1:B:491:LEU:HD21	1.95	0.48
1:A:361:GLU:N	1:A:362:PRO:HD2	2.28	0.48
1:A:407:THR:HB	1:A:409:ASP:OD1	2.14	0.48
1:B:280:LEU:CB	1:B:395:LEU:HD22	2.43	0.48
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.76	0.48
1:A:210:LEU:C	1:A:210:LEU:HD23	2.39	0.47
1:B:137:GLY:O	1:B:138:ALA:HB3	2.12	0.47
1:A:454:PHE:CD1	1:A:454:PHE:C	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HG21	1:B:469:VAL:CG2	2.42	0.47
1:A:367:LEU:O	1:A:371:ILE:HG13	2.14	0.47
1:B:441:ALA:O	1:B:445:LYS:HG3	2.15	0.47
1:A:142:VAL:HG12	1:A:265:ILE:HG22	1.97	0.47
1:B:90:ALA:HB1	1:B:95:PHE:O	2.16	0.46
1:B:302:GLY:O	1:B:303:MET:HB2	2.15	0.46
1:B:52:MET:O	1:B:54:PRO:HD3	2.15	0.46
1:B:63:VAL:CG1	1:B:423:LEU:HD11	2.25	0.46
1:B:312:ARG:NH2	1:B:410:GLU:OE1	2.49	0.46
1:B:28:ILE:O	1:B:32:VAL:HG22	2.14	0.46
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.99	0.46
1:B:177:LEU:HD12	1:B:177:LEU:C	2.41	0.46
1:B:188:THR:HB	1:B:189:PRO:CD	2.45	0.46
1:A:229:LYS:O	1:A:233:GLN:HG3	2.15	0.45
1:B:177:LEU:HB2	1:B:265:ILE:CG2	2.45	0.45
1:B:61:THR:HA	1:B:421:ALA:HB1	1.98	0.45
1:B:38:GLU:HB3	1:B:74:ILE:HD13	1.98	0.45
1:B:38:GLU:O	1:B:74:ILE:HD12	2.16	0.45
1:B:361:GLU:N	1:B:362:PRO:HD2	2.31	0.45
1:A:297:ARG:HH21	1:B:136:GLU:HA	1.80	0.45
1:A:201:GLU:HB3	1:A:264:LYS:HB2	1.99	0.45
1:A:137:GLY:O	1:A:138:ALA:HB3	2.16	0.45
1:A:244:TYR:CD2	1:B:183:ARG:HD2	2.52	0.45
1:B:61:THR:OG1	1:B:421:ALA:HB1	2.16	0.45
1:B:332:GLU:CB	1:B:333:PRO:HD2	2.43	0.45
1:A:357:LEU:CD1	1:A:368:TRP:HB2	2.47	0.45
1:B:60:PRO:HG2	1:B:106:SER:HB2	1.99	0.44
1:B:198:SER:O	1:B:240:HIS:HD2	1.99	0.44
1:A:280:LEU:HB3	1:A:395:LEU:HD22	1.98	0.44
1:B:114:ARG:NH2	1:B:511:ASP:OD2	2.46	0.44
1:B:280:LEU:HD12	1:B:281:ILE:N	2.32	0.44
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.43	0.44
1:B:188:THR:CB	1:B:189:PRO:CD	2.95	0.44
1:B:387:GLU:HA	1:B:396:ARG:NH2	2.32	0.44
1:B:395:LEU:O	1:B:399:ASP:N	2.50	0.44
1:A:425:PHE:HA	1:A:488:MET:HE1	1.99	0.44
1:B:367:LEU:O	1:B:371:ILE:HG13	2.18	0.44
1:A:114:ARG:HB2	1:A:507:LEU:HD22	1.99	0.44
1:B:9:PRO:HG3	1:B:21:PHE:CE2	2.53	0.44
1:B:230:PRO:HA	1:B:233:GLN:NE2	2.33	0.44
1:A:398:ARG:NH1	1:A:410:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLU:CD	1:B:224:GLU:H	2.25	0.44
1:B:314:ILE:HD12	1:B:342:ILE:HG22	2.01	0.43
1:B:516:THR:HG22	1:B:517:TYR:CD1	2.53	0.43
1:A:238:ILE:HG21	1:B:428:ILE:HG21	2.01	0.43
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.48	0.43
1:A:357:LEU:HD11	1:A:368:TRP:HB2	2.00	0.43
1:A:63:VAL:CG1	1:A:423:LEU:HD11	2.32	0.43
1:A:309:PRO:HB2	1:A:353:PHE:CE1	2.53	0.43
1:A:372:LYS:HG2	1:A:383:PHE:CZ	2.52	0.43
1:A:540:ILE:H	1:A:540:ILE:HG13	1.67	0.43
1:A:310:THR:O	1:A:353:PHE:HA	2.19	0.43
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.53	0.43
1:A:307:ASN:O	1:A:309:PRO:HD3	2.19	0.43
1:A:198:SER:O	1:A:240:HIS:HD2	2.01	0.43
1:B:74:ILE:HD12	1:B:74:ILE:N	2.33	0.43
1:A:63:VAL:HG11	1:A:423:LEU:CD1	2.32	0.43
1:B:258:ASN:HB2	1:B:541:ILE:O	2.19	0.43
1:A:244:TYR:O	1:A:245:GLY:C	2.62	0.42
1:B:177:LEU:HB2	1:B:265:ILE:HG21	2.01	0.42
1:B:398:ARG:NH1	1:B:410:GLU:OE2	2.50	0.42
1:A:314:ILE:HD12	1:A:342:ILE:HG22	2.01	0.42
1:A:324:LYS:HD2	1:A:416:TRP:NE1	2.34	0.42
1:B:100:ILE:HD13	1:B:111:ALA:HB1	2.01	0.42
1:B:417:LEU:HB3	1:B:418:PRO:CD	2.46	0.42
1:B:63:VAL:HG11	1:B:423:LEU:CD1	2.26	0.42
1:A:28:ILE:O	1:A:32:VAL:HG22	2.19	0.42
1:A:61:THR:HA	1:A:421:ALA:HB1	2.02	0.42
1:B:415:ASP:O	1:B:416:TRP:C	2.62	0.42
1:A:144:PRO:HD3	1:A:263:THR:O	2.20	0.42
1:B:210:LEU:HD23	1:B:211:ARG:N	2.35	0.42
1:B:493:ASP:O	1:B:494:ASP:C	2.61	0.42
1:A:93:PHE:O	1:A:94:SER:HB2	2.19	0.42
1:A:441:ALA:O	1:A:445:LYS:HG3	2.20	0.42
1:A:112:ALA:O	1:A:507:LEU:HD11	2.19	0.41
1:A:282:THR:HA	1:A:352:ASN:HD22	1.85	0.41
1:A:190:TYR:CD1	1:A:270:MET:HB2	2.56	0.41
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.55	0.41
1:B:109:GLY:O	1:B:110:GLY:C	2.64	0.41
1:B:431:VAL:HG22	1:B:465:MET:HG3	2.02	0.41
1:A:90:ALA:HB1	1:A:95:PHE:O	2.20	0.41
1:A:272:ASN:HA	1:A:273:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:PRO:HG2	1:A:460:VAL:HB	2.02	0.41
1:A:76:ALA:HA	1:A:77:PRO:HD2	1.92	0.41
1:A:302:GLY:O	1:A:303:MET:HB2	2.20	0.41
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.92	0.41
1:B:429:ALA:HB2	1:B:439:GLN:NE2	2.36	0.41
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.21	0.41
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.56	0.41
1:A:312:ARG:HD3	1:A:317:ASP:OD1	2.21	0.41
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.56	0.41
1:A:79:ASN:HD22	1:A:79:ASN:C	2.28	0.41
1:B:90:ALA:O	1:B:94:SER:N	2.54	0.41
1:B:464:GLU:OE1	1:B:466:HIS:ND1	2.47	0.41
1:B:503:TYR:O	1:B:504:ARG:HB2	2.20	0.41
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.56	0.41
1:B:131:LEU:HD12	1:B:141:VAL:HG12	2.03	0.41
1:B:238:ILE:HG22	1:B:238:ILE:O	2.22	0.40
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.56	0.40
1:A:138:ALA:O	1:B:463:ARG:NH2	2.50	0.40
1:A:231:GLU:H	1:A:231:GLU:HG3	1.30	0.40
1:B:197:HIS:HE1	1:B:251:ASP:OD2	2.05	0.40
1:A:210:LEU:HD23	1:A:211:ARG:N	2.36	0.40
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.57	0.40
1:A:310:THR:HG22	1:A:459:THR:HG22	2.03	0.40
1:B:210:LEU:HD23	1:B:210:LEU:C	2.46	0.40
1:B:132:GLU:O	1:B:140:CYS:HA	2.22	0.40

All (4) 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:A:18:LEU:CD2	1:A:30:ARG:NH1[3_655]	1.68	0.52
1:A:330:ARG:NH2	1:A:338:GLU:OE2[2_765]	1.71	0.49
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	2.04	0.16
1:B:18:LEU:CD2	1:B:30:ARG:NH1[4_565]	2.10	0.10

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	541/560 (97%)	504 (93%)	36 (7%)	1 (0%)	43	66
1	B	541/560 (97%)	506 (94%)	33 (6%)	2 (0%)	30	51
All	All	1082/1120 (97%)	1010 (93%)	69 (6%)	3 (0%)	36	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	PRO
1	B	67	ASP
1	B	418	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	466/481 (97%)	432 (93%)	34 (7%)	13	29
1	B	466/481 (97%)	430 (92%)	36 (8%)	12	27
All	All	932/962 (97%)	862 (92%)	70 (8%)	12	28

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	61	THR
1	A	62	HIS

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Mol	Chain	Res	Type
1	A	65	ASP
1	A	79	ASN
1	A	94	SER
1	A	106	SER
1	A	115	VAL
1	A	128	ASN
1	A	142	VAL
1	A	177	LEU
1	A	211	ARG
1	A	231	GLU
1	A	255	SER
1	A	265	ILE
1	A	297	ARG
1	A	301	LEU
1	A	303	MET
1	A	314	ILE
1	A	329	SER
1	A	331	THR
1	A	336	ASP
1	A	350	ARG
1	A	372	LYS
1	A	387	GLU
1	A	391	GLU
1	A	411	LEU
1	A	432	SER
1	A	457	THR
1	A	472	VAL
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	A	552	GLN
1	B	41	SER
1	B	61	THR
1	B	62	HIS
1	B	65	ASP
1	B	79	ASN
1	B	94	SER
1	B	106	SER
1	B	115	VAL
1	B	128	ASN
1	B	142	VAL
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	182	GLU
1	B	211	ARG
1	B	231	GLU
1	B	255	SER
1	B	290	LYS
1	B	297	ARG
1	B	301	LEU
1	B	303	MET
1	B	314	ILE
1	B	329	SER
1	B	331	THR
1	B	336	ASP
1	B	350	ARG
1	B	376	SER
1	B	387	GLU
1	B	391	GLU
1	B	411	LEU
1	B	432	SER
1	B	457	THR
1	B	462	MET
1	B	472	VAL
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	79	ASN
1	A	158	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	79	ASN
1	B	158	ASN
1	B	197	HIS
1	B	240	HIS

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Mol	Chain	Res	Type
1	B	352	ASN
1	B	439	GLN
1	B	467	HIS
1	B	485	GLN
1	B	520	ASN
1	B	552	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	B	600	-	28,29,29	1.61	5 (17%)	43,45,45	1.67	13 (30%)
2	ADP	A	600	-	28,29,29	1.58	5 (17%)	43,45,45	1.38	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	600	-	-	2/16/32/32	0/3/3/3
2	ADP	A	600	-	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	ADP	C5-N7	-4.42	1.31	1.39
2	B	600	ADP	C5-N7	-4.39	1.31	1.39
2	B	600	ADP	PB-O1B	4.19	1.63	1.50
2	A	600	ADP	PB-O1B	3.23	1.60	1.50
2	B	600	ADP	C8-N7	-2.65	1.26	1.31
2	B	600	ADP	C2-N1	2.62	1.38	1.33
2	A	600	ADP	O4'-C1'	-2.29	1.36	1.42
2	A	600	ADP	C2-N1	2.28	1.38	1.33
2	A	600	ADP	PA-O3A	2.21	1.61	1.59
2	B	600	ADP	PB-O2B	-2.03	1.47	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	ADP	C6-C5-N7	-3.17	125.98	132.09
2	B	600	ADP	O4'-C1'-N9	3.11	114.07	108.09
2	A	600	ADP	C4-N9-C8	-3.01	102.57	105.74
2	B	600	ADP	C4-C5-N7	2.97	113.97	110.58
2	A	600	ADP	C2'-C3'-C4'	-2.81	97.19	102.61
2	B	600	ADP	O2B-PB-O3A	2.69	113.67	104.64
2	A	600	ADP	O3A-PB-O1B	-2.67	97.00	111.04
2	B	600	ADP	C4-N9-C8	-2.57	103.04	105.74
2	A	600	ADP	O2'-C2'-C3'	-2.47	103.89	111.82
2	B	600	ADP	O2A-PA-O5'	2.39	118.40	107.57
2	B	600	ADP	O3A-PB-O1B	-2.38	98.53	111.04
2	B	600	ADP	N9-C8-N7	2.37	117.30	113.94
2	A	600	ADP	O2B-PB-O3A	2.36	112.54	104.64
2	B	600	ADP	C4-N9-C1'	2.35	132.13	126.63
2	B	600	ADP	C5-C4-N9	-2.34	103.26	105.81
2	B	600	ADP	N6-C6-N1	2.28	123.46	118.38
2	A	600	ADP	O2A-PA-O5'	2.23	117.69	107.57
2	A	600	ADP	PA-O5'-C5'	2.18	133.82	121.35
2	B	600	ADP	O2A-PA-O3A	2.14	113.06	107.27
2	B	600	ADP	C6-C5-C4	2.10	120.05	117.18
2	A	600	ADP	C4-C5-N7	2.00	112.87	110.58

There are no chirality outliers.

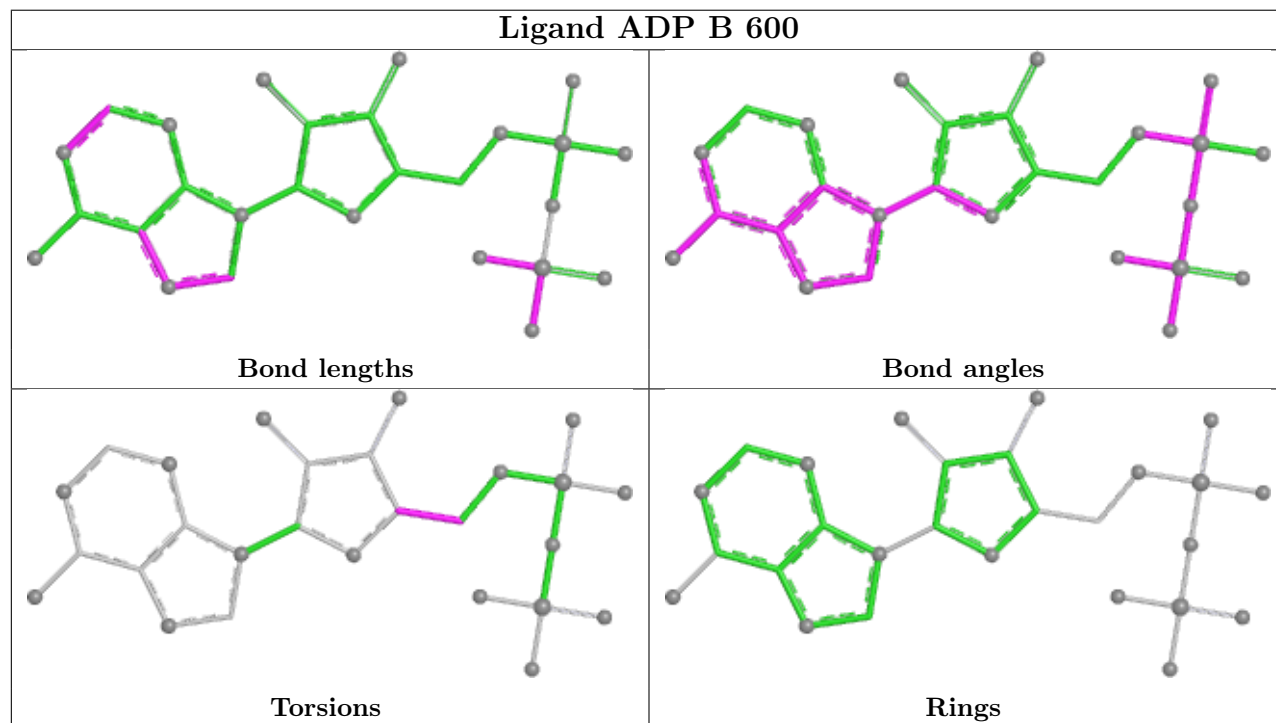
All (4) torsion outliers are listed below:

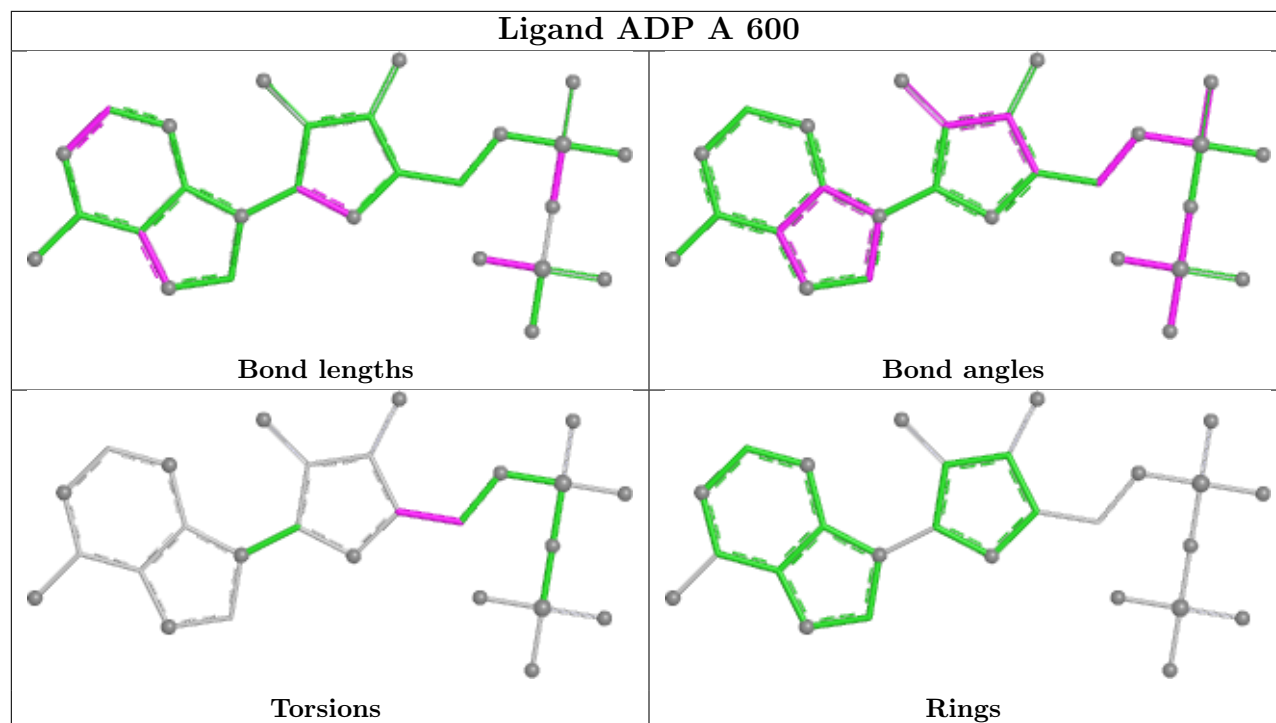
Mol	Chain	Res	Type	Atoms
2	A	600	ADP	O4'-C4'-C5'-O5'
2	A	600	ADP	C3'-C4'-C5'-O5'
2	B	600	ADP	O4'-C4'-C5'-O5'
2	B	600	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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	545/560 (97%)	0.00	6 (1%) 78 74	20, 42, 64, 78	27 (4%)
1	B	545/560 (97%)	0.02	8 (1%) 72 68	20, 42, 64, 78	27 (4%)
All	All	1090/1120 (97%)	0.01	14 (1%) 75 71	20, 42, 64, 78	54 (4%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	HIS	2.8
1	A	62	HIS	2.8
1	B	6	GLU	2.7
1	A	61	THR	2.7
1	B	61	THR	2.5
1	A	63	VAL	2.4
1	A	24	PHE	2.4
1	A	322	GLY	2.4
1	A	6	GLU	2.3
1	B	24	PHE	2.3
1	B	7	PHE	2.2
1	B	391	GLU	2.1
1	B	331	THR	2.1
1	B	54	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

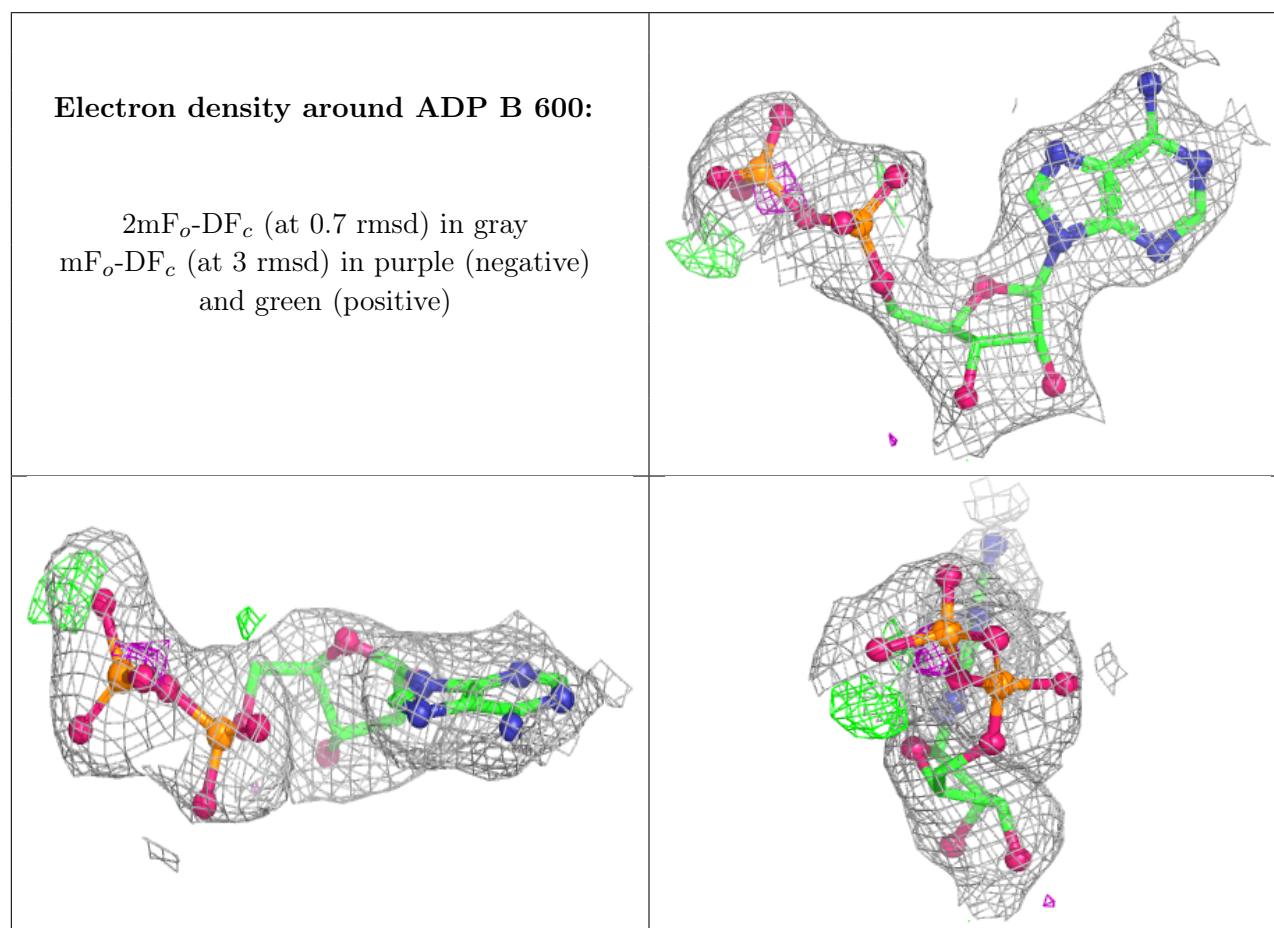
There are no oligosaccharides in this entry.

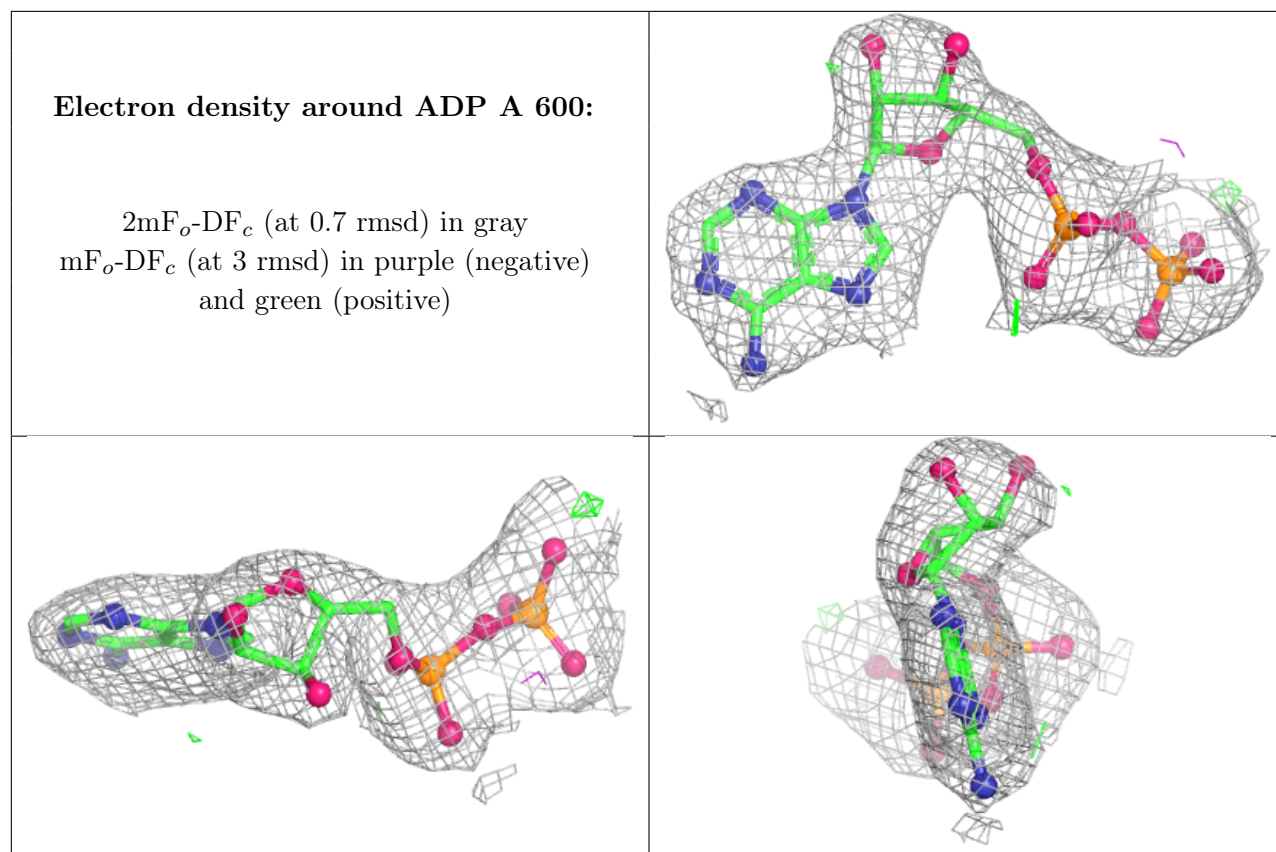
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	B	600	27/27	0.88	0.10	47,50,61,63	0
2	ADP	A	600	27/27	0.91	0.09	47,50,61,63	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.