



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:54 AM UTC

PDB ID : 1E4E / pdb_00001e4e
Title : D-alanyl-D-lacate ligase
Authors : Roper, D.I.
Deposited on : 2000-07-03
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

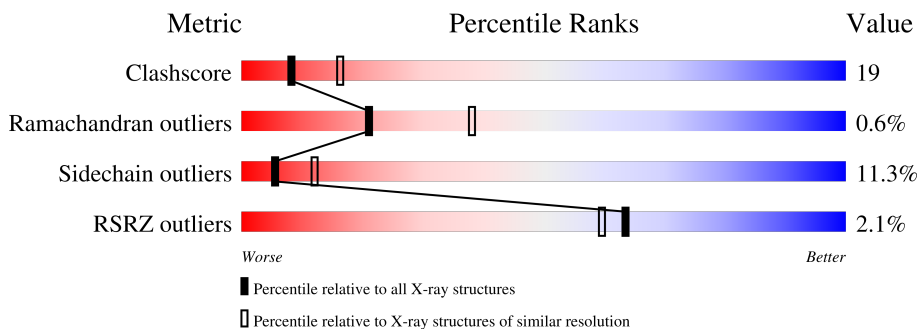
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	
2	B	343	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	1344	-	-	X	-
7	GOL	A	1345	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	1346	-	X	X	-
7	GOL	A	1348	-	-	X	-
7	GOL	A	990	-	-	X	-
7	GOL	B	1345	-	X	-	-
7	GOL	B	1346	-	-	X	-
7	GOL	B	1347	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5750 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 VANCOMYCIN/TEICoplanin A-TYPE RESISTANCE PROTEIN VANA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2607	1653	443	496	15	5	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GLU	ASP	conflict	UNP P25051
A	276	VAL	ALA	conflict	UNP P25051
A	282	THR	ALA	conflict	UNP P25051
A	328	SER	ALA	conflict	UNP P25051

- Molecule 2 is a protein called VANCOMYCIN/TEICoplanin A-TYPE RESISTANCE PROTEIN VANA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	340	2603	1650	446	492	15	33	0	0

There are 5 discrepancies between the modelled and reference sequences:

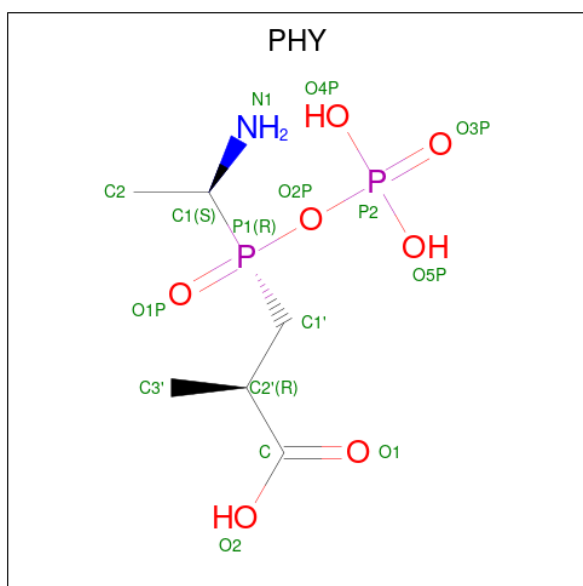
Chain	Residue	Modelled	Actual	Comment	Reference
B	62	GLU	ASP	conflict	UNP P25051
B	276	VAL	ALA	conflict	UNP P25051
B	282	THR	ALA	conflict	UNP P25051
B	298	ARG	ASN	conflict	UNP P25051
B	328	SER	ALA	conflict	UNP P25051

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



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

- Molecule 4 is 1(S)-AMINOETHYL-(2-CARBOXYPROPYL)PHOSPHORYL-PHOSPHINI C ACID (CCD ID: PHY) (formula: C₆H₁₅NO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			14	5	1	6	2		

Continued on next page...

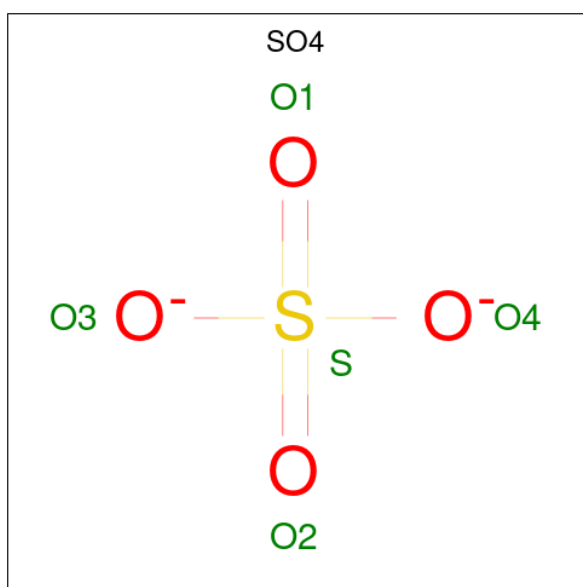
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			14	5	1	6	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	B	2	Total	Mg	0	0
			2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

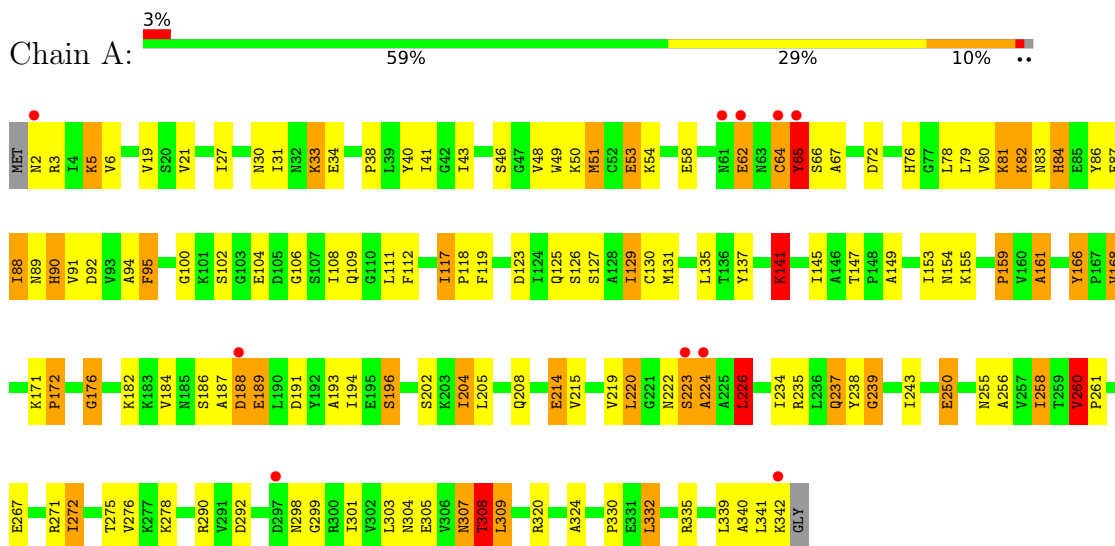
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	169	Total O 169 169	0	0
8	A	1	Total O 1 1	0	0
8	A	2	Total O 2 2	0	0
8	A	3	Total O 3 3	0	0
8	B	173	Total O 173 173	0	0
8	B	1	Total O 1 1	0	0
8	B	1	Total O 1 1	0	0
8	B	5	Total O 5 5	0	0

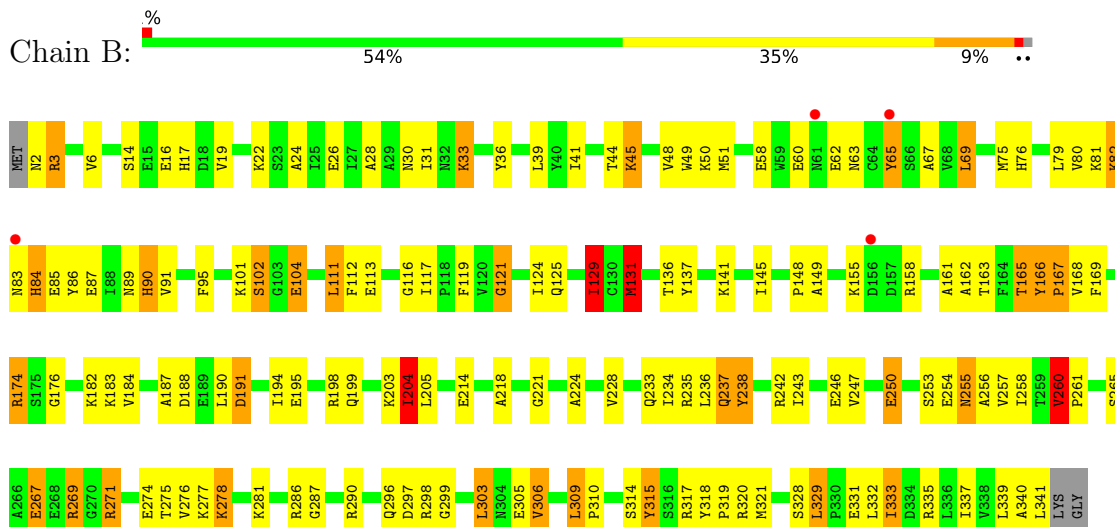
3 Residue-property plots i

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: VANCOMYCIN/TEICOPLANIN A-TYPE RESISTANCE PROTEIN VANA



- Molecule 2: VANCOMYCIN/TEICOPLANIN A-TYPE RESISTANCE PROTEIN VANA



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.20Å 225.36Å 72.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.3 (15.00-2.50) 92.8 (15.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.88 (at 2.51Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.257 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtrriage
Anisotropy	0.476	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5750	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PHY, MG, SO4, GOL, 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	1.77	37/2654 (1.4%)	1.76	45/3589 (1.3%)
2	B	1.84	33/2650 (1.2%)	1.83	64/3583 (1.8%)
All	All	1.80	70/5304 (1.3%)	1.80	109/7172 (1.5%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLN	CA-CB	-23.34	1.16	1.53
2	B	84	HIS	CA-CB	20.91	1.90	1.53
2	B	62	GLU	CA-CB	-18.54	1.24	1.53
2	B	155	LYS	CB-CG	-13.74	1.11	1.52
2	B	58	GLU	CA-CB	-10.53	1.38	1.53
1	A	147	THR	N-CA	-9.20	1.38	1.46
2	B	82	LYS	CG-CD	-8.43	1.27	1.52
1	A	154	ASN	CA-C	-8.07	1.41	1.53
1	A	147	THR	C-O	-7.31	1.17	1.24
1	A	65	TYR	N-CA	7.03	1.54	1.46
1	A	88	ILE	C-O	-6.86	1.17	1.24
1	A	341	LEU	CA-C	6.78	1.61	1.52
2	B	238	TYR	C-O	6.65	1.30	1.23
1	A	51	MET	SD-CE	-6.59	1.63	1.79
1	A	95	PHE	N-CA	-6.55	1.38	1.46
2	B	6	VAL	CA-CB	6.45	1.61	1.53
1	A	250	GLU	CD-OE1	6.43	1.37	1.25
1	A	194	ILE	CA-CB	6.35	1.61	1.54
2	B	48	VAL	CA-CB	6.32	1.62	1.54
1	A	341	LEU	C-O	-6.30	1.16	1.24
2	B	149	ALA	CA-CB	-6.25	1.44	1.53
1	A	83	ASN	CA-C	-6.21	1.45	1.53
1	A	194	ILE	C-O	6.20	1.31	1.24
1	A	332	LEU	C-O	6.07	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	ILE	CA-C	-6.03	1.45	1.52
1	A	147	THR	CA-CB	6.03	1.61	1.53
2	B	306	VAL	CA-CB	-5.99	1.46	1.54
1	A	64	CYS	C-O	-5.97	1.16	1.24
1	A	342	LYS	CA-CB	5.95	1.65	1.53
2	B	183	LYS	CE-NZ	5.91	1.67	1.49
2	B	276	VAL	CA-CB	5.86	1.61	1.54
2	B	315	TYR	CA-C	5.85	1.60	1.52
1	A	341	LEU	N-CA	5.78	1.53	1.46
1	A	176	GLY	C-O	5.73	1.29	1.23
1	A	214	GLU	CA-C	-5.71	1.45	1.52
2	B	165	THR	CA-C	5.57	1.59	1.52
2	B	24	ALA	C-O	5.55	1.31	1.24
2	B	238	TYR	CA-C	-5.44	1.46	1.52
1	A	130	CYS	CA-C	5.42	1.60	1.52
2	B	275	THR	CA-CB	-5.42	1.44	1.53
2	B	306	VAL	CB-CG2	5.42	1.70	1.52
1	A	278	LYS	CA-C	5.39	1.59	1.52
1	A	108	ILE	CA-CB	5.36	1.60	1.54
2	B	85	GLU	CA-CB	5.34	1.67	1.53
1	A	21	VAL	CA-C	5.34	1.59	1.52
1	A	149	ALA	CA-CB	5.34	1.62	1.53
2	B	305	GLU	CD-OE2	-5.32	1.15	1.25
2	B	148	PRO	C-O	-5.31	1.17	1.23
2	B	129	ILE	CG1-CD1	5.30	1.72	1.51
2	B	194	ILE	CA-CB	-5.30	1.47	1.54
1	A	324	ALA	C-O	-5.26	1.17	1.24
2	B	333	ILE	CA-CB	-5.22	1.48	1.54
2	B	22	LYS	C-O	-5.20	1.18	1.24
2	B	31	ILE	CA-CB	-5.20	1.48	1.54
1	A	46	SER	N-CA	-5.18	1.40	1.46
1	A	191	ASP	CA-C	-5.17	1.46	1.52
1	A	342	LYS	N-CA	5.17	1.56	1.46
2	B	199	GLN	CG-CD	5.16	1.65	1.52
2	B	131	MET	SD-CE	-5.15	1.66	1.79
1	A	90	HIS	C-O	-5.09	1.17	1.23
2	B	204	ILE	CA-C	-5.09	1.46	1.52
1	A	6	VAL	CA-C	5.08	1.59	1.52
2	B	224	ALA	C-O	-5.05	1.17	1.24
1	A	256	ALA	C-O	-5.04	1.17	1.24
2	B	190	LEU	CA-CB	-5.04	1.45	1.53
1	A	102	SER	CA-C	-5.04	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	MET	SD-CE	-5.02	1.67	1.79
2	B	191	ASP	CA-C	-5.02	1.46	1.52
1	A	21	VAL	C-O	5.00	1.29	1.24
2	B	278	LYS	CA-C	-5.00	1.45	1.52

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	84	HIS	N-CA-CB	19.17	138.87	110.49
2	B	62	GLU	CB-CA-C	14.06	134.58	110.68
1	A	65	TYR	N-CA-C	12.29	129.31	109.76
2	B	158	ARG	CB-CG-CD	11.97	138.84	111.30
1	A	208	GLN	N-CA-CB	11.90	127.58	109.85
1	A	208	GLN	CG-CD-NE2	-11.50	99.15	116.40
1	A	208	GLN	CA-CB-CG	9.60	133.30	114.10
1	A	340	ALA	CA-C-O	9.31	130.68	119.97
2	B	269	ARG	NE-CZ-NH2	-8.13	111.88	119.20
2	B	191	ASP	N-CA-C	8.10	119.89	111.14
1	A	250	GLU	CB-CG-CD	7.96	126.13	112.60
2	B	84	HIS	CA-CB-CG	-7.74	106.06	113.80
1	A	208	GLN	CB-CG-CD	7.71	125.71	112.60
2	B	335	ARG	NE-CZ-NH2	-7.70	112.27	119.20
1	A	208	GLN	CB-CA-C	7.47	121.85	109.89
2	B	62	GLU	N-CA-CB	-7.47	98.85	110.06
2	B	183	LYS	CA-C-N	-7.44	113.45	123.12
2	B	183	LYS	C-N-CA	-7.44	113.45	123.12
1	A	208	GLN	CG-CD-OE1	7.29	135.38	120.80
2	B	131	MET	CB-CG-SD	7.24	134.41	112.70
1	A	64	CYS	CA-CB-SG	-7.14	97.99	114.40
2	B	155	LYS	CA-CB-CG	7.11	128.32	114.10
2	B	269	ARG	NE-CZ-NH1	7.05	128.55	121.50
2	B	199	GLN	N-CA-C	-7.05	104.15	112.89
2	B	340	ALA	N-CA-C	-6.96	103.69	111.28
1	A	141	LYS	CA-CB-CG	6.95	128.00	114.10
2	B	167	PRO	N-CD-CG	-6.90	95.52	103.80
1	A	260	VAL	CB-CA-C	-6.87	98.86	111.36
1	A	308	THR	N-CA-CB	-6.84	100.03	110.16
1	A	307	ASN	CA-C-O	6.82	127.75	120.46
1	A	341	LEU	O-C-N	-6.77	113.98	122.17
2	B	187	ALA	N-CA-C	6.75	119.47	111.71
1	A	64	CYS	N-CA-C	6.56	124.77	110.80
2	B	124	ILE	N-CA-C	6.41	116.57	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	298	ARG	N-CA-C	-6.40	104.58	112.38
2	B	317	ARG	N-CA-C	6.38	118.31	111.36
1	A	320	ARG	NE-CZ-NH2	-6.29	113.54	119.20
2	B	90	HIS	N-CA-C	6.27	119.08	110.24
2	B	161	ALA	N-CA-C	6.22	118.06	111.28
2	B	19	VAL	N-CA-C	-6.20	104.30	110.62
1	A	309	LEU	CA-CB-CG	-6.16	94.75	116.30
1	A	308	THR	CB-CA-C	6.12	121.25	110.85
2	B	104	GLU	CA-C-N	-6.11	112.89	122.73
2	B	104	GLU	C-N-CA	-6.11	112.89	122.73
1	A	34	GLU	N-CA-C	-6.10	103.96	111.40
2	B	260	VAL	CB-CA-C	-6.09	100.27	111.36
2	B	33	LYS	CD-CE-NZ	6.09	131.39	111.90
2	B	163	THR	CA-C-N	-6.09	112.13	122.67
2	B	163	THR	C-N-CA	-6.09	112.13	122.67
2	B	221	GLY	N-CA-C	6.08	118.22	112.08
2	B	145	ILE	N-CA-C	-6.07	99.67	108.17
1	A	141	LYS	CB-CA-C	6.07	120.40	110.88
1	A	250	GLU	CG-CD-OE1	5.96	132.10	118.40
1	A	127	SER	N-CA-C	-5.96	104.71	111.14
1	A	40	TYR	N-CA-C	5.93	117.86	108.67
1	A	342	LYS	N-CA-C	5.91	127.56	111.00
2	B	45	LYS	CA-C-N	-5.91	113.20	122.65
2	B	45	LYS	C-N-CA	-5.91	113.20	122.65
2	B	81	LYS	CB-CG-CD	5.91	124.89	111.30
2	B	267	GLU	N-CA-C	-5.88	104.46	111.69
2	B	121	GLY	N-CA-C	5.88	122.45	112.22
1	A	78	LEU	N-CA-C	5.87	119.24	110.14
2	B	116	GLY	N-CA-C	-5.87	107.14	115.30
2	B	166	TYR	CB-CA-C	5.86	117.94	109.09
2	B	129	ILE	N-CA-C	5.82	118.36	111.09
1	A	64	CYS	N-CA-CB	-5.82	100.66	110.49
1	A	298	ASN	N-CA-CB	-5.82	100.21	110.39
2	B	257	VAL	CB-CA-C	-5.79	102.55	110.77
2	B	174	ARG	N-CA-C	5.77	118.01	108.49
1	A	272	ILE	N-CA-C	-5.75	104.73	111.00
2	B	84	HIS	N-CA-C	-5.72	105.96	113.17
2	B	149	ALA	N-CA-C	-5.69	100.40	109.96
1	A	19	VAL	N-CA-C	-5.67	103.84	111.44
1	A	226	LEU	N-CA-C	5.66	122.86	110.80
1	A	21	VAL	N-CA-C	-5.63	105.01	110.42
2	B	79	LEU	N-CA-C	-5.61	98.20	108.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	GLY	N-CA-C	5.61	121.43	111.73
2	B	129	ILE	CG1-CB-CG2	-5.55	94.04	110.70
2	B	271	ARG	NE-CZ-NH2	-5.55	114.21	119.20
2	B	3	ARG	NE-CZ-NH2	-5.47	114.27	119.20
2	B	129	ILE	CA-CB-CG1	5.44	119.65	110.40
1	A	243	ILE	N-CA-C	5.44	116.82	110.62
2	B	30	ASN	CA-C-N	-5.39	113.41	120.91
2	B	30	ASN	C-N-CA	-5.39	113.41	120.91
1	A	6	VAL	N-CA-C	5.39	115.34	107.37
2	B	58	GLU	CB-CA-C	5.38	118.62	111.14
1	A	196	SER	CB-CA-C	5.38	119.40	110.90
1	A	161	ALA	N-CA-C	5.37	117.13	111.28
1	A	117	ILE	N-CA-CB	5.35	115.06	110.08
2	B	183	LYS	N-CA-C	-5.34	101.08	109.25
2	B	3	ARG	CD-NE-CZ	5.31	131.83	124.40
2	B	41	ILE	N-CA-C	5.25	114.86	106.88
2	B	237	GLN	N-CA-C	-5.23	106.40	112.89
1	A	159	PRO	CA-C-O	-5.21	115.06	121.31
1	A	65	TYR	CB-CA-C	-5.20	101.37	109.84
2	B	162	ALA	N-CA-C	-5.17	106.07	112.38
1	A	166	TYR	CB-CA-C	5.16	116.29	108.86
1	A	172	PRO	CA-C-O	-5.16	115.58	121.56
1	A	168	VAL	CB-CA-C	5.16	119.94	110.71
2	B	113	GLU	N-CA-CB	5.16	117.48	110.01
2	B	85	GLU	N-CA-C	5.14	117.83	109.24
1	A	72	ASP	N-CA-C	5.10	117.06	109.25
2	B	310	PRO	N-CD-CG	-5.10	95.55	103.20
1	A	145	ILE	CB-CA-C	-5.06	104.27	111.21
2	B	298	ARG	CD-NE-CZ	-5.05	117.33	124.40
2	B	84	HIS	CB-CA-C	-5.02	101.71	110.09
2	B	44	THR	N-CA-CB	5.01	117.10	110.29
2	B	67	ALA	CA-C-N	-5.00	115.24	122.45
2	B	67	ALA	C-N-CA	-5.00	115.24	122.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2607	0	2602	102	4
2	B	2603	0	2607	92	0
3	A	27	0	12	3	0
3	B	27	0	12	2	0
4	A	14	0	5	4	0
4	B	14	0	6	4	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	10	0	0	4	0
6	B	5	0	0	1	0
7	A	48	0	61	12	4
7	B	36	0	48	14	0
8	A	175	0	0	6	0
8	B	180	0	0	17	0
All	All	5750	0	5353	206	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 19.

All (206) 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:A:51:MET:O	1:A:65:TYR:N	1.77	1.17
2:B:314:SER:HA	7:B:1347:GOL:H31	1.36	1.06
1:A:51:MET:HE2	1:A:65:TYR:CD2	1.92	1.05
4:B:355:PHY:P1	4:B:355:PHY:C2	2.45	1.04
2:B:286:ARG:HD2	8:B:2149:HOH:O	1.59	1.01
4:A:355:PHY:C2	4:A:355:PHY:N1	2.25	1.00
1:A:141:LYS:HE3	8:B:2075:HOH:O	1.62	0.99
4:A:355:PHY:C2	4:A:355:PHY:P1	2.52	0.97
1:A:51:MET:HB3	1:A:65:TYR:HB2	1.47	0.96
2:B:26:GLU:OE1	7:B:1347:GOL:O2	1.83	0.95
2:B:271:ARG:NH2	2:B:299:GLY:O	2.02	0.92
4:B:355:PHY:C2	4:B:355:PHY:N1	2.34	0.90
1:A:335:ARG:O	1:A:339:LEU:HD13	1.73	0.88
6:A:1344:SO4:O4	8:B:3009:HOH:O	1.92	0.85
1:A:239:GLY:H	7:A:1346:GOL:H11	1.40	0.84
2:B:50:LYS:NZ	2:B:60:GLU:OE2	2.11	0.83
1:A:223:SER:O	1:A:224:ALA:HB3	1.76	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:355:PHY:N1	4:A:355:PHY:P1	2.52	0.82
2:B:89:ASN:CB	7:B:1346:GOL:O3	2.27	0.82
2:B:89:ASN:HB3	7:B:1346:GOL:O3	1.80	0.81
4:B:355:PHY:P1	4:B:355:PHY:N1	2.53	0.81
1:A:51:MET:HE2	1:A:65:TYR:CE2	2.19	0.78
2:B:26:GLU:HB3	7:B:1347:GOL:O2	1.84	0.78
6:A:1344:SO4:O1	8:B:3010:HOH:O	2.03	0.77
6:A:1344:SO4:S	8:B:3009:HOH:O	2.42	0.77
2:B:83:ASN:CG	2:B:84:HIS:H	1.92	0.76
1:A:271:ARG:NH2	1:A:299:GLY:O	2.19	0.76
2:B:250:GLU:H	2:B:250:GLU:CD	1.95	0.75
2:B:265:SER:HB2	8:B:2137:HOH:O	1.86	0.75
1:A:51:MET:HB3	1:A:65:TYR:CB	2.19	0.72
1:A:238:TYR:HB2	7:A:1346:GOL:H11	1.72	0.71
2:B:237:GLN:HG3	2:B:238:TYR:CD2	2.26	0.71
1:A:223:SER:O	1:A:224:ALA:CB	2.39	0.70
2:B:125:GLN:O	2:B:129:ILE:HG23	1.91	0.70
1:A:3:ARG:HG3	7:A:1348:GOL:H12	1.71	0.70
1:A:308:THR:CG2	8:A:2076:HOH:O	2.40	0.70
6:A:1344:SO4:O1	8:B:3009:HOH:O	2.10	0.69
2:B:2:ASN:HB2	8:B:2001:HOH:O	1.90	0.69
2:B:255:ASN:HD22	2:B:255:ASN:H	1.42	0.68
2:B:168:VAL:O	2:B:184:VAL:N	2.22	0.67
2:B:51:MET:HE1	7:B:1346:GOL:H2	1.74	0.67
1:A:82:LYS:HD3	1:A:87:GLU:HG2	1.77	0.66
2:B:218:ALA:HB1	2:B:318:TYR:CD2	2.31	0.65
1:A:239:GLY:H	7:A:1346:GOL:C1	2.10	0.65
2:B:50:LYS:HE2	7:B:1348:GOL:O2	1.98	0.64
2:B:69:LEU:HD21	2:B:117:ILE:HD12	1.78	0.64
1:A:50:LYS:HA	1:A:65:TYR:O	1.97	0.64
1:A:137:TYR:O	1:A:141:LYS:HB3	1.98	0.63
2:B:318:TYR:N	2:B:319:PRO:HD2	2.14	0.62
1:A:123:ASP:HB2	8:A:2066:HOH:O	1.99	0.62
1:A:88:ILE:C	1:A:89:ASN:HD22	2.08	0.62
1:A:304:ASN:ND2	8:A:2151:HOH:O	2.32	0.62
1:A:308:THR:HG23	8:A:2076:HOH:O	2.01	0.61
1:A:51:MET:C	1:A:65:TYR:H	1.98	0.60
2:B:296:GLN:O	2:B:299:GLY:N	2.33	0.60
4:B:355:PHY:H1'2	4:B:355:PHY:O3P	2.01	0.60
1:A:33:LYS:HE2	1:A:38:PRO:HG3	1.84	0.59
2:B:39:LEU:HD22	7:B:1346:GOL:H2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:SER:HA	7:B:1347:GOL:C3	2.24	0.58
2:B:83:ASN:CG	2:B:84:HIS:N	2.62	0.57
1:A:215:VAL:HG21	1:A:272:ILE:HD13	1.85	0.57
1:A:84:HIS:HE1	7:A:1347:GOL:H2	1.68	0.57
1:A:84:HIS:CE1	7:A:1347:GOL:H2	2.40	0.57
2:B:76:HIS:O	2:B:76:HIS:CD2	2.58	0.57
2:B:236:LEU:HD23	2:B:256:ALA:HB2	1.85	0.56
1:A:95:PHE:C	1:A:95:PHE:CD1	2.83	0.56
1:A:51:MET:CE	1:A:65:TYR:CE2	2.87	0.56
1:A:153:ILE:HD12	1:A:159:PRO:HG3	1.87	0.56
1:A:155:LYS:HD2	1:A:202:SER:HB2	1.88	0.56
1:A:51:MET:O	1:A:64:CYS:C	2.48	0.56
1:A:182:LYS:HD3	1:A:193:ALA:HB2	1.87	0.56
1:A:106:GLY:HA2	1:A:109:GLN:OE1	2.05	0.56
2:B:236:LEU:CD2	2:B:256:ALA:HB2	2.36	0.55
1:A:90:HIS:HE1	1:A:92:ASP:OD1	1.89	0.55
2:B:195:GLU:OE2	2:B:198:ARG:NH1	2.40	0.55
1:A:3:ARG:HE	7:A:1348:GOL:H12	1.72	0.54
2:B:328:SER:HB3	8:B:2168:HOH:O	2.06	0.54
1:A:129:ILE:HA	1:A:135:LEU:HD23	1.90	0.54
2:B:75:MET:O	2:B:76:HIS:C	2.49	0.54
1:A:226:LEU:H	1:A:226:LEU:HD13	1.72	0.54
1:A:234:ILE:HG12	1:A:258:ILE:HG12	1.91	0.53
1:A:260:VAL:HA	1:A:261:PRO:C	2.31	0.53
1:A:76:HIS:CD2	1:A:76:HIS:O	2.61	0.53
2:B:314:SER:CA	7:B:1347:GOL:H31	2.25	0.53
1:A:53:GLU:HG2	1:A:54:LYS:HG2	1.91	0.53
2:B:17:HIS:ND1	2:B:45:LYS:HG2	2.24	0.53
2:B:243:ILE:HD13	2:B:253:SER:HB2	1.90	0.52
2:B:2:ASN:N	8:B:2001:HOH:O	2.41	0.52
1:A:51:MET:CB	1:A:65:TYR:HB2	2.30	0.52
4:A:355:PHY:O3P	4:A:355:PHY:H1'2	2.09	0.52
2:B:36:TYR:CE1	2:B:337:ILE:HG21	2.45	0.52
2:B:218:ALA:HB1	2:B:318:TYR:CE2	2.45	0.52
1:A:238:TYR:HB2	7:A:1346:GOL:C1	2.40	0.52
2:B:45:LYS:HG3	8:B:2021:HOH:O	2.10	0.52
2:B:51:MET:HE1	7:B:1346:GOL:C2	2.39	0.52
1:A:31:ILE:HG23	1:A:33:LYS:HE3	1.92	0.51
2:B:233:GLN:O	2:B:258:ILE:HA	2.11	0.51
2:B:204:ILE:C	2:B:204:ILE:HD12	2.36	0.51
2:B:203:LYS:HE2	6:B:1342:SO4:O4	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:HA	7:A:1348:GOL:O1	2.11	0.51
2:B:17:HIS:CE1	2:B:45:LYS:HG2	2.45	0.51
1:A:89:ASN:N	1:A:89:ASN:ND2	2.59	0.50
1:A:100:GLY:N	1:A:104:GLU:OE1	2.39	0.50
1:A:222:ASN:O	1:A:223:SER:C	2.54	0.50
2:B:104:GLU:O	2:B:131:MET:HG2	2.11	0.50
1:A:222:ASN:O	1:A:223:SER:O	2.28	0.50
2:B:214:GLU:HB2	2:B:234:ILE:HB	1.94	0.50
1:A:81:LYS:HB2	1:A:86:TYR:CE1	2.46	0.50
1:A:89:ASN:HD22	1:A:89:ASN:N	2.10	0.50
1:A:95:PHE:C	1:A:95:PHE:HD1	2.20	0.50
1:A:43:ILE:HA	1:A:48:VAL:O	2.12	0.49
1:A:76:HIS:CD2	1:A:91:VAL:O	2.65	0.49
2:B:166:TYR:HB3	2:B:167:PRO:HA	1.95	0.49
2:B:131:MET:HE3	2:B:174:ARG:HB3	1.93	0.49
1:A:65:TYR:O	1:A:66:SER:C	2.54	0.49
1:A:125:GLN:O	1:A:129:ILE:HG12	2.13	0.49
2:B:137:TYR:O	2:B:141:LYS:HG3	2.12	0.48
1:A:112:PHE:HB3	1:A:119:PHE:CD2	2.49	0.48
2:B:76:HIS:O	2:B:76:HIS:HD2	1.96	0.48
1:A:161:ALA:HB1	1:A:187:ALA:HB1	1.96	0.48
2:B:303:LEU:HD21	2:B:306:VAL:HG23	1.94	0.48
1:A:204:ILE:C	1:A:204:ILE:HD12	2.38	0.47
2:B:65:TYR:HB2	8:B:2043:HOH:O	2.14	0.47
2:B:182:LYS:HB3	2:B:182:LYS:HE2	1.59	0.47
1:A:188:ASP:OD1	1:A:188:ASP:N	2.43	0.47
1:A:5:LYS:HE2	7:A:1350:GOL:H31	1.96	0.46
2:B:14:SER:HA	8:B:2004:HOH:O	2.14	0.46
2:B:242:ARG:O	2:B:243:ILE:C	2.57	0.46
2:B:121:GLY:HA2	2:B:287:GLY:HA3	1.97	0.46
2:B:129:ILE:HD12	2:B:129:ILE:HG21	1.49	0.46
2:B:218:ALA:O	2:B:228:VAL:HA	2.16	0.46
1:A:65:TYR:N	1:A:65:TYR:CD1	2.84	0.46
1:A:76:HIS:HD2	1:A:91:VAL:O	1.99	0.45
2:B:260:VAL:HA	2:B:261:PRO:C	2.41	0.45
2:B:274:GLU:O	2:B:278:LYS:HG2	2.16	0.45
2:B:90:HIS:ND1	8:B:2048:HOH:O	2.36	0.45
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.83	0.45
2:B:250:GLU:CD	2:B:250:GLU:N	2.68	0.45
2:B:318:TYR:N	2:B:319:PRO:CD	2.80	0.45
1:A:214:GLU:OE2	3:A:350:ADP:O2'	2.26	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TYR:HD2	1:A:80:VAL:CG1	2.30	0.44
2:B:125:GLN:NE2	8:B:2069:HOH:O	2.50	0.44
2:B:188:ASP:OD1	2:B:188:ASP:N	2.44	0.44
1:A:58:GLU:HA	8:A:2030:HOH:O	2.17	0.44
1:A:51:MET:HB3	1:A:65:TYR:CG	2.53	0.44
1:A:76:HIS:O	1:A:76:HIS:HD2	2.00	0.44
2:B:76:HIS:CD2	2:B:91:VAL:O	2.71	0.44
1:A:62:GLU:HA	1:A:62:GLU:OE1	2.17	0.44
1:A:219:VAL:HG12	1:A:220:LEU:N	2.32	0.44
2:B:16:GLU:O	2:B:17:HIS:C	2.59	0.44
1:A:129:ILE:HG22	1:A:135:LEU:HD21	2.00	0.43
1:A:3:ARG:HG3	7:A:1348:GOL:C1	2.45	0.43
1:A:126:SER:HA	1:A:129:ILE:HG12	2.00	0.43
2:B:234:ILE:HG12	2:B:258:ILE:HG12	1.99	0.43
1:A:260:VAL:CA	1:A:261:PRO:C	2.90	0.43
2:B:49:TRP:CZ3	2:B:69:LEU:HB2	2.53	0.43
1:A:239:GLY:N	7:A:1346:GOL:H11	2.21	0.43
1:A:186:SER:O	1:A:189:GLU:HG3	2.19	0.43
2:B:176:GLY:HA2	3:B:350:ADP:O1B	2.19	0.43
1:A:49:TRP:HB3	1:A:67:ALA:O	2.19	0.43
1:A:275:THR:O	1:A:276:VAL:C	2.61	0.43
2:B:3:ARG:CD	2:B:33:LYS:O	2.67	0.43
2:B:112:PHE:HB3	2:B:119:PHE:CD1	2.54	0.43
1:A:226:LEU:N	1:A:226:LEU:CD1	2.82	0.43
1:A:104:GLU:HG2	1:A:308:THR:HG22	2.01	0.42
1:A:88:ILE:C	1:A:89:ASN:ND2	2.76	0.42
1:A:176:GLY:HA2	3:A:350:ADP:O1B	2.19	0.42
1:A:226:LEU:H	1:A:226:LEU:CD1	2.32	0.42
2:B:236:LEU:HD23	2:B:256:ALA:CB	2.48	0.42
2:B:290:ARG:HD2	2:B:321:MET:HE1	2.02	0.42
2:B:309:LEU:HD22	2:B:309:LEU:HA	1.94	0.42
1:A:82:LYS:HZ2	1:A:87:GLU:CD	2.28	0.42
2:B:129:ILE:HG23	2:B:129:ILE:HD13	1.65	0.42
1:A:237:GLN:HG3	1:A:238:TYR:CD2	2.55	0.42
1:A:292:ASP:HB3	1:A:304:ASN:HD22	1.85	0.42
1:A:51:MET:O	1:A:64:CYS:HA	2.20	0.41
2:B:80:VAL:O	2:B:86:TYR:HA	2.20	0.41
2:B:269:ARG:HD2	8:B:2141:HOH:O	2.20	0.41
2:B:297:ASP:C	2:B:299:GLY:N	2.76	0.41
2:B:246:GLU:OE1	2:B:254:GLU:N	2.40	0.41
2:B:315:TYR:O	2:B:320:ARG:NH1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HB2	1:A:172:PRO:HD2	2.02	0.41
1:A:292:ASP:O	1:A:304:ASN:HB3	2.20	0.41
2:B:39:LEU:CD1	7:B:1346:GOL:H31	2.50	0.41
1:A:129:ILE:HD12	1:A:129:ILE:HG21	1.54	0.41
2:B:111:LEU:O	2:B:112:PHE:C	2.64	0.41
1:A:65:TYR:N	1:A:65:TYR:HD1	2.18	0.41
1:A:214:GLU:OE2	3:A:350:ADP:H2'	2.21	0.41
1:A:290:ARG:HH11	1:A:290:ARG:HD3	1.62	0.41
2:B:89:ASN:HB2	7:B:1346:GOL:O3	2.19	0.41
2:B:329:LEU:O	2:B:333:ILE:HG13	2.21	0.41
1:A:51:MET:N	1:A:65:TYR:O	2.45	0.41
1:A:94:ALA:O	1:A:119:PHE:HA	2.21	0.41
1:A:166:TYR:CZ	1:A:187:ALA:HA	2.54	0.41
2:B:218:ALA:CB	2:B:318:TYR:CD2	3.00	0.41
2:B:238:TYR:CZ	2:B:255:ASN:HB3	2.54	0.41
2:B:277:LYS:HE2	8:B:2144:HOH:O	2.21	0.41
2:B:329:LEU:HD23	2:B:329:LEU:HA	1.73	0.41
1:A:275:THR:HG21	1:A:301:ILE:HG21	2.03	0.41
2:B:50:LYS:HE2	7:B:1348:GOL:C2	2.50	0.41
2:B:169:PHE:CE1	3:B:350:ADP:C2	3.09	0.40
2:B:28:ALA:O	2:B:33:LYS:NZ	2.45	0.40
1:A:307:ASN:HB3	8:A:2154:HOH:O	2.21	0.40
2:B:297:ASP:C	2:B:299:GLY:H	2.28	0.40
1:A:30:ASN:HB3	1:A:330:PRO:HG3	2.03	0.40
1:A:117:ILE:HG22	1:A:118:PRO:O	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:64:CYS:O	7:A:990:GOL:O2[6_555]	1.83	0.37
1:A:65:TYR:CA	7:A:990:GOL:C1[6_555]	1.92	0.28
1:A:64:CYS:C	7:A:990:GOL:O2[6_555]	1.96	0.24
1:A:64:CYS:O	7:A:990:GOL:C2[6_555]	2.09	0.11

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	339/343 (99%)	319 (94%)	17 (5%)	3 (1%)	14	27
2	B	338/343 (98%)	322 (95%)	15 (4%)	1 (0%)	36	55
All	All	677/686 (99%)	641 (95%)	32 (5%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	A	224	ALA
2	B	102	SER
1	A	226	LEU

5.3.2 Protein sidechains [i](#)

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	279/285 (98%)	246 (88%)	33 (12%)	5	11
2	B	279/285 (98%)	249 (89%)	30 (11%)	6	13
All	All	558/570 (98%)	495 (89%)	63 (11%)	5	12

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	33	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	41	ILE
1	A	53	GLU
1	A	62	GLU
1	A	65	TYR
1	A	81	LYS
1	A	82	LYS
1	A	84	HIS
1	A	111	LEU
1	A	129	ILE
1	A	141	LYS
1	A	168	VAL
1	A	184	VAL
1	A	188	ASP
1	A	189	GLU
1	A	196	SER
1	A	204	ILE
1	A	205	LEU
1	A	220	LEU
1	A	226	LEU
1	A	235	ARG
1	A	237	GLN
1	A	250	GLU
1	A	255	ASN
1	A	258	ILE
1	A	260	VAL
1	A	267	GLU
1	A	303	LEU
1	A	305	GLU
1	A	308	THR
1	A	309	LEU
1	A	332	LEU
2	B	63	ASN
2	B	65	TYR
2	B	69	LEU
2	B	82	LYS
2	B	87	GLU
2	B	95	PHE
2	B	101	LYS
2	B	102	SER
2	B	111	LEU
2	B	129	ILE
2	B	131	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	136	THR
2	B	165	THR
2	B	191	ASP
2	B	204	ILE
2	B	205	LEU
2	B	235	ARG
2	B	247	VAL
2	B	250	GLU
2	B	255	ASN
2	B	260	VAL
2	B	267	GLU
2	B	281	LYS
2	B	303	LEU
2	B	309	LEU
2	B	329	LEU
2	B	331	GLU
2	B	332	LEU
2	B	339	LEU
2	B	341	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	30	ASN
1	A	76	HIS
1	A	84	HIS
1	A	89	ASN
1	A	90	HIS
1	A	199	GLN
1	A	237	GLN
1	A	255	ASN
1	A	304	ASN
2	B	30	ASN
2	B	76	HIS
2	B	125	GLN
2	B	142	ASN
2	B	199	GLN
2	B	255	ASN
2	B	304	ASN

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 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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
6	SO4	B	1342	-	4,4,4	0.49	0	6,6,6	0.83	0
7	GOL	B	1348	-	5,5,5	0.45	0	5,5,5	0.58	0
7	GOL	B	1347	-	5,5,5	0.65	0	5,5,5	1.07	1 (20%)
7	GOL	B	1346	-	5,5,5	0.41	0	5,5,5	0.53	0
7	GOL	A	1345	-	5,5,5	1.62	1 (20%)	5,5,5	3.12	3 (60%)
4	PHY	B	355	5	5,11,15	1.06	1 (20%)	5,14,23	1.63	1 (20%)
7	GOL	A	1347	-	5,5,5	0.64	0	5,5,5	0.84	0
7	GOL	B	1345	-	5,5,5	0.38	0	5,5,5	2.07	3 (60%)
3	ADP	B	350	5	28,29,29	1.35	4 (14%)	43,45,45	1.76	11 (25%)
7	GOL	B	1344	-	5,5,5	0.36	0	5,5,5	0.34	0
6	SO4	A	1343	-	4,4,4	0.13	0	6,6,6	1.35	1 (16%)
3	ADP	A	350	5	28,29,29	1.31	4 (14%)	43,45,45	1.67	11 (25%)
7	GOL	A	1348	-	5,5,5	0.53	0	5,5,5	2.26	3 (60%)
7	GOL	A	1349	-	5,5,5	0.49	0	5,5,5	0.40	0
7	GOL	A	990	-	5,5,5	0.52	0	5,5,5	1.83	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	1344	-	4,4,4	0.39	0	6,6,6	0.38	0
7	GOL	A	1350	-	5,5,5	0.48	0	5,5,5	0.37	0
7	GOL	A	996	-	5,5,5	0.58	0	5,5,5	0.49	0
7	GOL	A	1346	-	5,5,5	1.04	0	5,5,5	2.31	2 (40%)
7	GOL	B	1343	-	5,5,5	0.31	0	5,5,5	1.52	1 (20%)
4	PHY	A	355	5	5,11,15	2.56	2 (40%)	5,14,23	3.45	3 (60%)

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	350	5	-	6/16/32/32	0/3/3/3
7	GOL	A	1347	-	-	4/4/4/4	-
7	GOL	A	1349	-	-	2/4/4/4	-
7	GOL	A	990	-	-	1/4/4/4	-
7	GOL	B	1348	-	-	4/4/4/4	-
7	GOL	B	1345	-	-	3/4/4/4	-
7	GOL	A	996	-	-	4/4/4/4	-
7	GOL	B	1347	-	-	2/4/4/4	-
7	GOL	B	1344	-	-	2/4/4/4	-
7	GOL	B	1346	-	-	4/4/4/4	-
7	GOL	A	1345	-	-	3/4/4/4	-
3	ADP	A	350	5	-	3/16/32/32	0/3/3/3
7	GOL	A	1350	-	-	2/4/4/4	-
7	GOL	A	1348	-	-	1/4/4/4	-
7	GOL	A	1346	-	-	4/4/4/4	-
7	GOL	B	1343	-	-	2/4/4/4	-
4	PHY	B	355	5	-	2/5/12/21	-
4	PHY	A	355	5	-	3/5/12/21	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	355	PHY	C2'-C	4.44	1.64	1.51
4	A	355	PHY	O1-C	-3.17	1.12	1.22
3	A	350	ADP	C2-N1	3.13	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	350	ADP	C2-N3	3.05	1.39	1.33
3	B	350	ADP	C2-N1	2.84	1.39	1.33
7	A	1345	GOL	O2-C2	-2.82	1.35	1.43
3	A	350	ADP	PB-O3B	-2.67	1.44	1.54
3	B	350	ADP	C3'-C4'	-2.60	1.46	1.53
3	A	350	ADP	O3'-C3'	-2.26	1.37	1.43
3	B	350	ADP	C6-N6	-2.11	1.28	1.34
3	A	350	ADP	O4'-C1'	2.07	1.46	1.42
4	B	355	PHY	C2'-C	2.01	1.57	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	355	PHY	O2-C-O1	6.09	137.90	124.08
7	A	1345	GOL	O2-C2-C3	-4.81	89.25	109.18
7	A	1345	GOL	C3-C2-C1	-4.31	95.98	111.80
3	A	350	ADP	N3-C2-N1	-4.22	122.20	128.58
3	B	350	ADP	N3-C2-N1	-4.05	122.45	128.58
3	B	350	ADP	N9-C8-N7	-3.84	108.49	113.94
3	A	350	ADP	O2A-PA-O3A	3.73	117.36	107.27
3	B	350	ADP	O2A-PA-O3A	3.72	117.32	107.27
4	A	355	PHY	O1-C-C2'	-3.41	111.89	122.27
7	A	1346	GOL	O2-C2-C3	-3.40	95.12	109.18
7	A	1346	GOL	O3-C3-C2	-3.33	95.40	110.38
3	B	350	ADP	O5'-C5'-C4'	3.28	120.17	108.99
3	A	350	ADP	O3B-PB-O3A	3.24	115.50	104.64
3	A	350	ADP	N9-C8-N7	-3.02	109.65	113.94
3	A	350	ADP	C5-C4-N3	-3.01	122.57	126.72
7	A	1348	GOL	C3-C2-C1	2.90	122.45	111.80
3	B	350	ADP	O3B-PB-O2B	2.89	118.64	107.80
4	A	355	PHY	C1'-C2'-C	2.88	115.59	110.33
7	B	1345	GOL	O2-C2-C1	2.83	120.89	109.18
3	B	350	ADP	C5-C4-N3	-2.82	122.83	126.72
7	A	1348	GOL	O2-C2-C3	2.74	120.54	109.18
7	B	1345	GOL	O3-C3-C2	-2.71	98.19	110.38
3	B	350	ADP	C4-N9-C8	2.69	108.56	105.74
3	B	350	ADP	C2-N3-C4	2.66	118.33	111.83
3	B	350	ADP	C5-N7-C8	2.63	107.58	103.45
7	B	1343	GOL	O2-C2-C3	2.58	119.85	109.18
7	A	1345	GOL	O2-C2-C1	-2.50	98.82	109.18
3	A	350	ADP	C2-N3-C4	2.40	117.69	111.83
3	B	350	ADP	C5'-C4'-C3'	-2.39	106.59	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	355	PHY	C1'-C2'-C	2.37	114.66	110.33
7	A	1348	GOL	O3-C3-C2	2.31	120.78	110.38
6	A	1343	SO4	O3-S-O1	-2.28	97.66	109.56
7	A	990	GOL	O3-C3-C2	2.27	120.61	110.38
3	B	350	ADP	N3-C4-N9	2.27	131.03	127.17
7	B	1347	GOL	O3-C3-C2	2.23	120.43	110.38
3	A	350	ADP	C5-N7-C8	2.16	106.85	103.45
3	A	350	ADP	O3A-PA-O1A	-2.15	104.23	110.70
3	A	350	ADP	O3B-PB-O2B	2.14	115.84	107.80
7	A	990	GOL	C3-C2-C1	2.09	119.48	111.80
3	A	350	ADP	C3'-C2'-C1'	-2.09	97.50	101.46
7	A	990	GOL	O2-C2-C1	2.07	117.75	109.18
7	B	1345	GOL	O2-C2-C3	2.05	117.67	109.18
3	A	350	ADP	C2'-C3'-C4'	2.02	106.50	102.61

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	350	ADP	PA-O3A-PB-O2B
3	B	350	ADP	PA-O3A-PB-O2B
3	B	350	ADP	PA-O3A-PB-O3B
7	A	1346	GOL	O1-C1-C2-C3
7	A	1349	GOL	O1-C1-C2-C3
7	A	996	GOL	C1-C2-C3-O3
7	B	1343	GOL	C1-C2-C3-O3
7	B	1345	GOL	C1-C2-C3-O3
7	B	1345	GOL	O2-C2-C3-O3
7	B	1346	GOL	C1-C2-C3-O3
7	B	1347	GOL	O1-C1-C2-C3
7	B	1348	GOL	O1-C1-C2-C3
7	A	1345	GOL	O2-C2-C3-O3
7	A	1345	GOL	O1-C1-C2-C3
7	A	1345	GOL	C1-C2-C3-O3
7	A	1346	GOL	C1-C2-C3-O3
7	A	1347	GOL	O1-C1-C2-C3
7	A	1347	GOL	C1-C2-C3-O3
7	A	1350	GOL	C1-C2-C3-O3
7	A	996	GOL	O1-C1-C2-C3
7	B	1344	GOL	O1-C1-C2-C3
7	B	1345	GOL	O1-C1-C2-C3
7	B	1346	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	1348	GOL	C1-C2-C3-O3
7	A	1347	GOL	O1-C1-C2-O2
7	A	1349	GOL	O1-C1-C2-O2
7	A	996	GOL	O1-C1-C2-O2
7	B	1343	GOL	O2-C2-C3-O3
7	B	1346	GOL	O1-C1-C2-O2
7	B	1347	GOL	O1-C1-C2-O2
7	B	1348	GOL	O1-C1-C2-O2
7	A	1346	GOL	O2-C2-C3-O3
7	A	996	GOL	O2-C2-C3-O3
7	B	1344	GOL	O1-C1-C2-O2
7	B	1346	GOL	O2-C2-C3-O3
7	B	1348	GOL	O2-C2-C3-O3
7	A	1347	GOL	O2-C2-C3-O3
3	B	350	ADP	O4'-C4'-C5'-O5'
7	A	1346	GOL	O1-C1-C2-O2
7	A	1350	GOL	O2-C2-C3-O3
4	A	355	PHY	P1-C1'-C2'-C3'
4	A	355	PHY	O1-C-C2'-C1'
4	B	355	PHY	O2-C-C2'-C1'
7	A	1348	GOL	O2-C2-C3-O3
3	A	350	ADP	C4'-C5'-O5'-PA
3	B	350	ADP	PB-O3A-PA-O1A
3	B	350	ADP	PB-O3A-PA-O2A
3	A	350	ADP	PA-O3A-PB-O3B
7	A	990	GOL	O2-C2-C3-O3
3	B	350	ADP	C3'-C4'-C5'-O5'
4	A	355	PHY	O2-C-C2'-C1'
4	B	355	PHY	O1-C-C2'-C1'

There are no ring outliers.

14 monomers are involved in 48 short contacts:

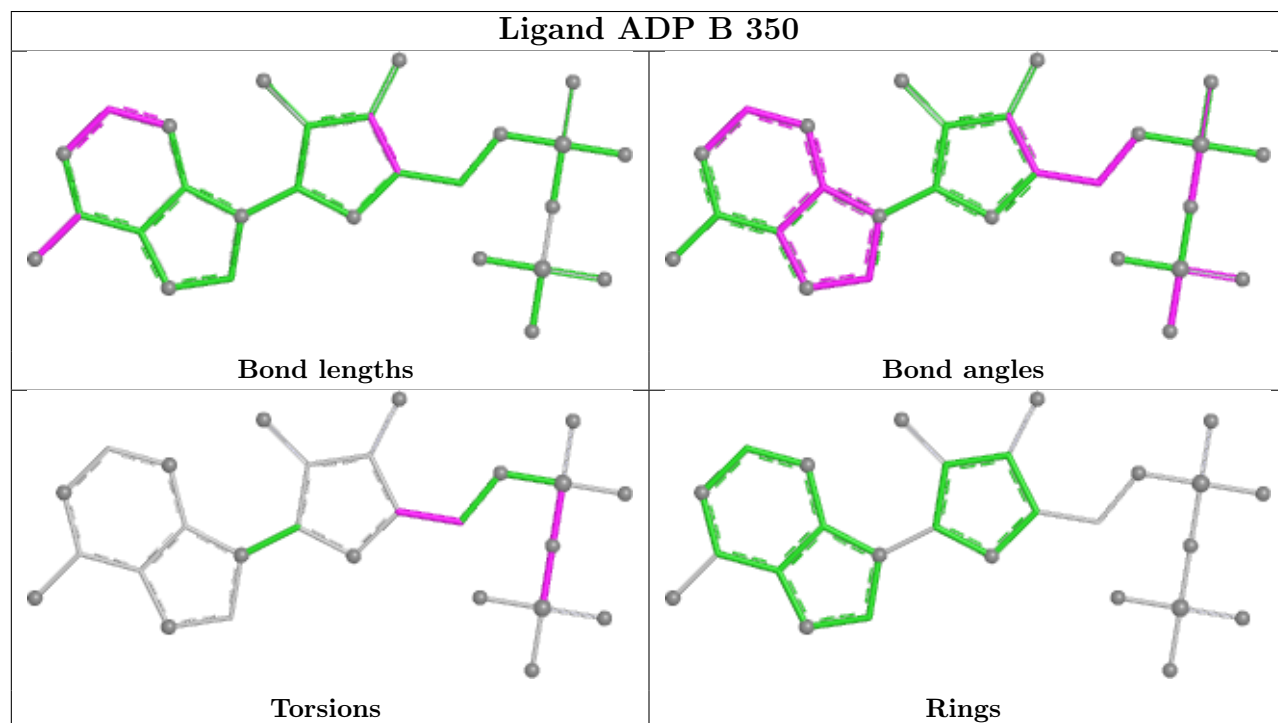
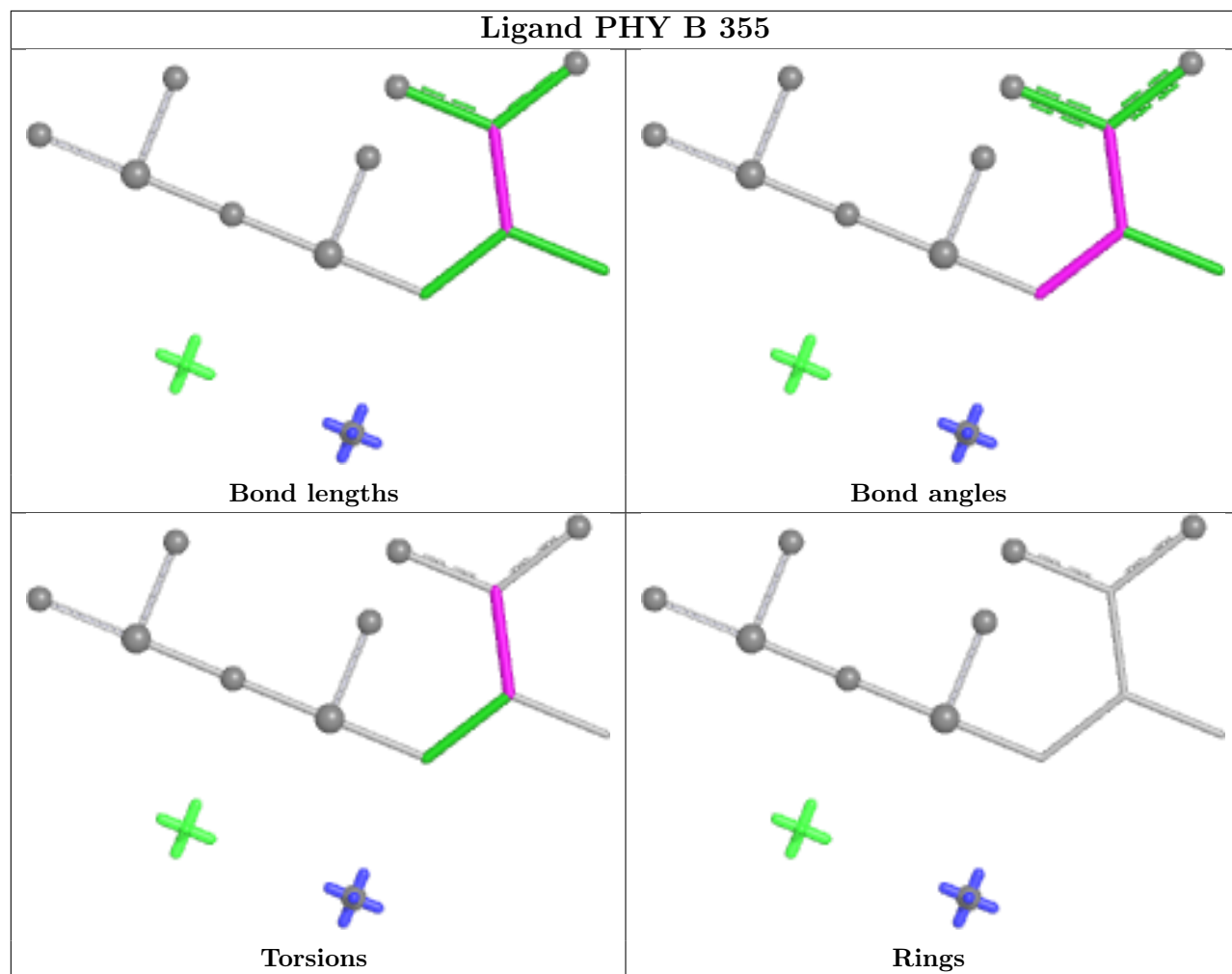
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1342	SO4	1	0
7	B	1348	GOL	2	0
7	B	1347	GOL	5	0
7	B	1346	GOL	7	0
4	B	355	PHY	4	0
7	A	1347	GOL	2	0
3	B	350	ADP	2	0
3	A	350	ADP	3	0

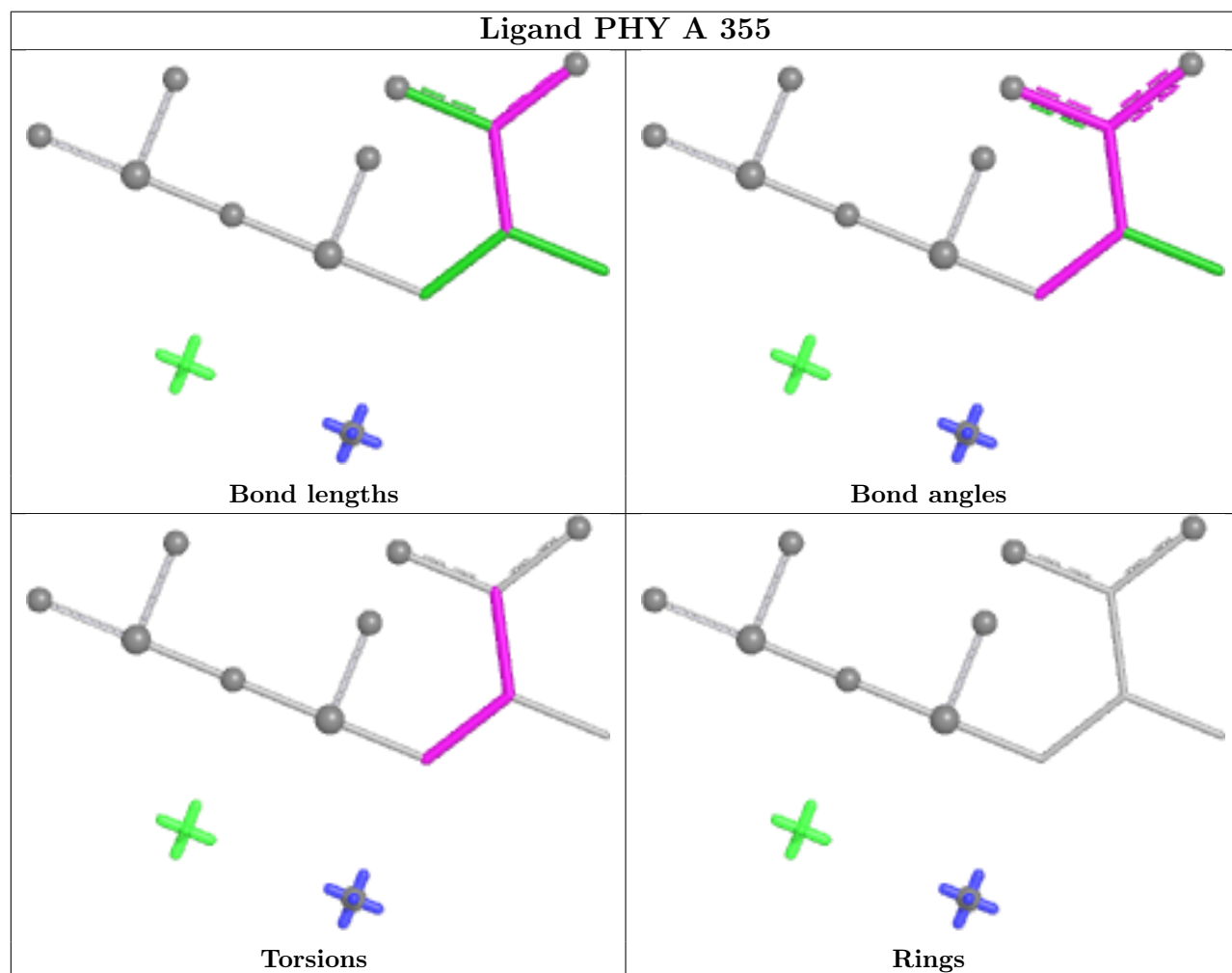
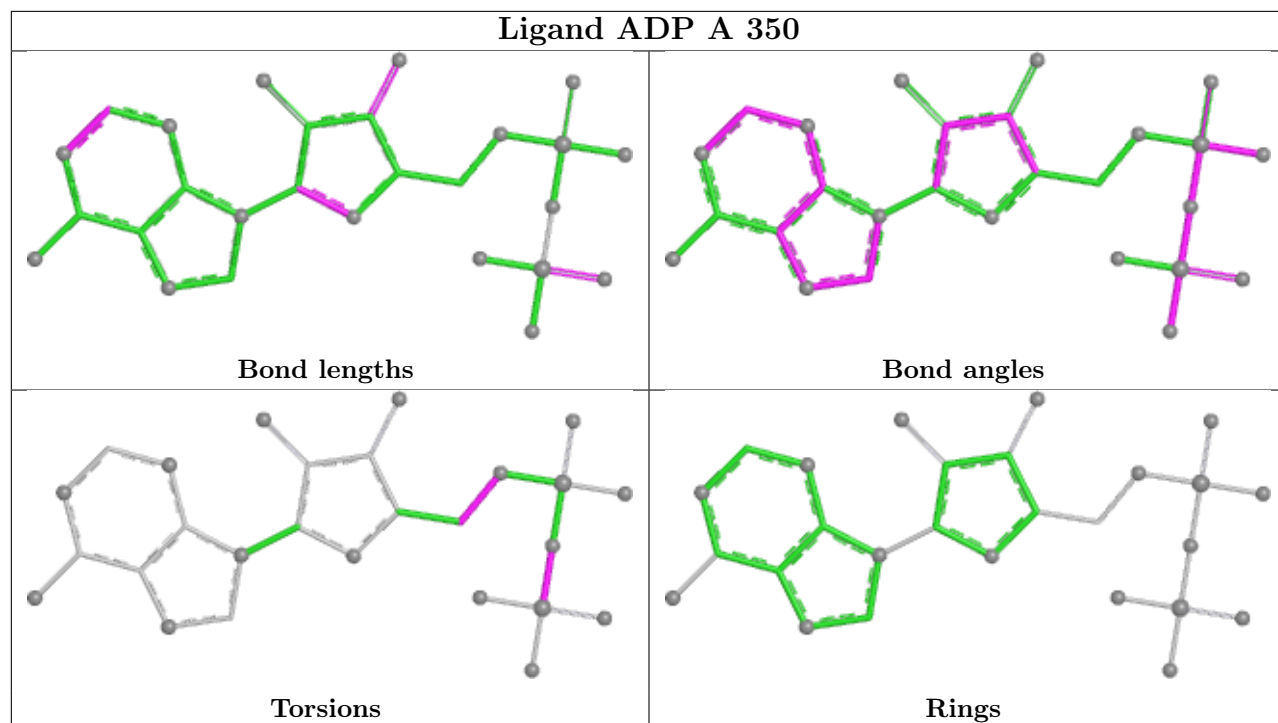
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1348	GOL	4	0
7	A	990	GOL	0	4
6	A	1344	SO4	4	0
7	A	1350	GOL	1	0
7	A	1346	GOL	5	0
4	A	355	PHY	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/343 (99%)	-0.25	10 (2%) 53 49	23, 52, 72, 88	1 (0%)
2	B	340/343 (99%)	-0.29	4 (1%) 76 73	28, 49, 69, 86	8 (2%)
All	All	681/686 (99%)	-0.27	14 (2%) 63 59	23, 51, 72, 88	9 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	TYR	5.7
2	B	83	ASN	3.1
1	A	64	CYS	3.1
1	A	61	ASN	2.9
2	B	65	TYR	2.8
2	B	156	ASP	2.7
2	B	61	ASN	2.6
1	A	297	ASP	2.5
1	A	2	ASN	2.4
1	A	188	ASP	2.4
1	A	62	GLU	2.3
1	A	223	SER	2.1
1	A	342	LYS	2.1
1	A	224	ALA	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

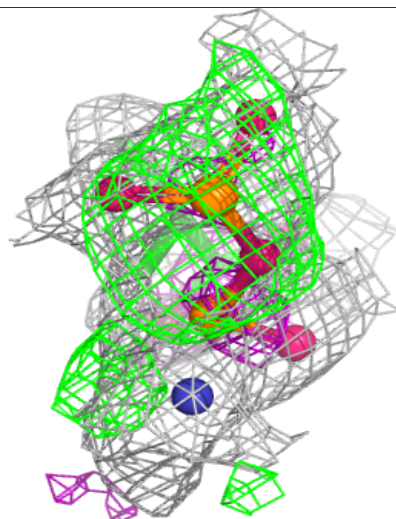
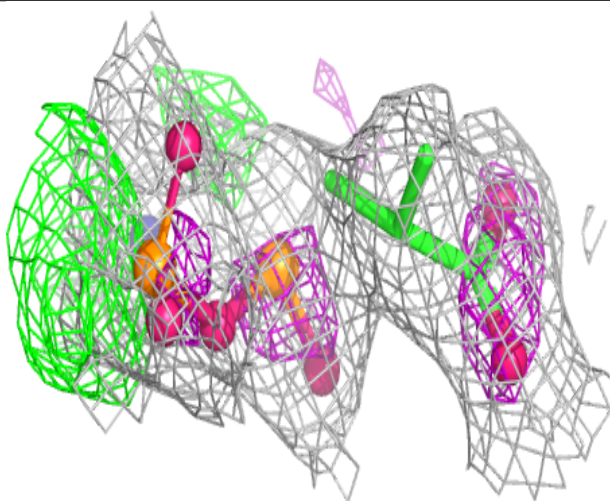
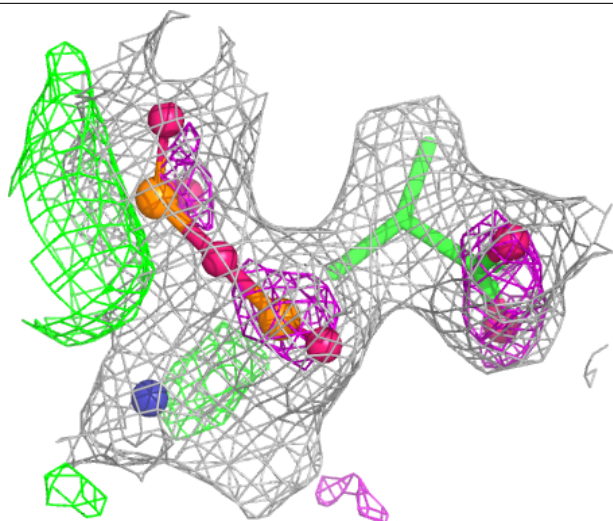
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	996	6/6	0.60	0.16	116,117,118,119	0
7	GOL	A	1349	6/6	0.72	0.21	106,108,109,109	0
7	GOL	A	1350	6/6	0.73	0.22	125,126,126,127	0
7	GOL	B	1345	6/6	0.75	0.17	68,72,73,74	0
7	GOL	B	1348	6/6	0.76	0.17	92,94,94,94	0
7	GOL	B	1346	6/6	0.77	0.23	95,100,101,103	0
7	GOL	B	1343	6/6	0.77	0.15	99,101,102,103	0
7	GOL	B	1344	6/6	0.82	0.18	104,107,108,112	0
7	GOL	A	990	6/6	0.85	0.23	73,80,85,92	0
7	GOL	A	1348	6/6	0.86	0.15	83,84,85,87	0
5	MG	A	360	1/1	0.88	0.13	46,46,46,46	0
7	GOL	A	1347	6/6	0.89	0.16	61,67,74,80	0
7	GOL	A	1345	6/6	0.90	0.14	47,57,62,66	0
5	MG	B	360	1/1	0.90	0.07	42,42,42,42	0
7	GOL	A	1346	6/6	0.92	0.12	71,72,73,73	0
7	GOL	B	1347	6/6	0.92	0.17	82,84,87,88	0
6	SO4	A	1344	5/5	0.92	0.19	93,96,98,98	0
4	PHY	B	355	14/16	0.93	0.12	33,35,39,39	0
4	PHY	A	355	14/16	0.94	0.10	34,40,42,44	0
6	SO4	A	1343	5/5	0.96	0.12	56,59,62,65	0
5	MG	B	365	1/1	0.97	0.09	38,38,38,38	0
6	SO4	B	1342	5/5	0.97	0.11	50,54,56,57	0
3	ADP	A	350	27/27	0.98	0.06	41,47,51,52	0
3	ADP	B	350	27/27	0.98	0.06	33,45,50,51	0
5	MG	A	365	1/1	0.99	0.03	42,42,42,42	0

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

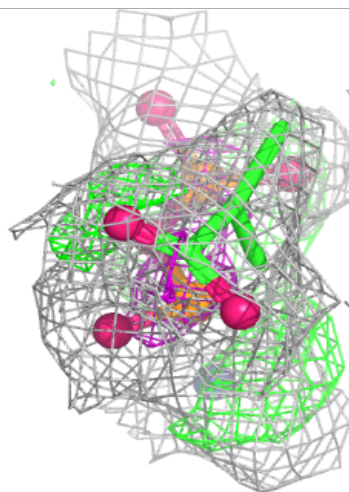
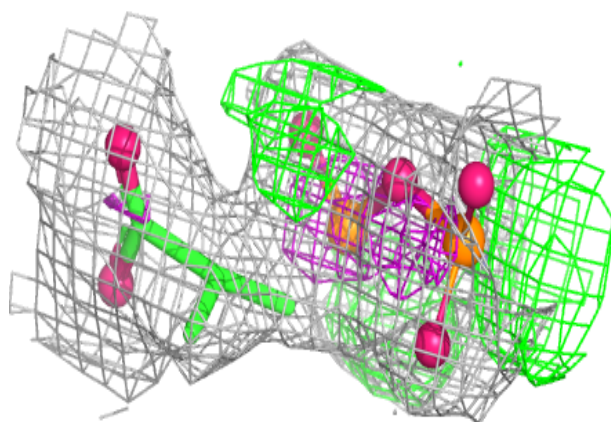
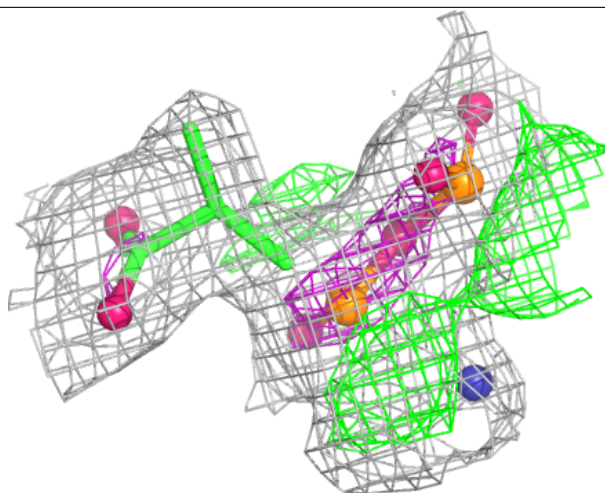
Electron density around PHY B 355:

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



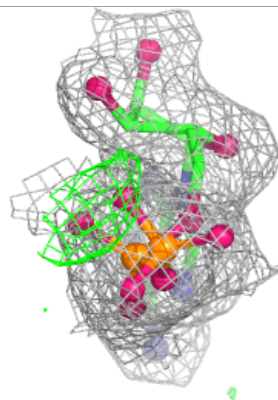
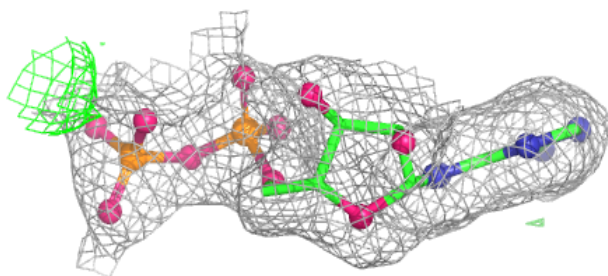
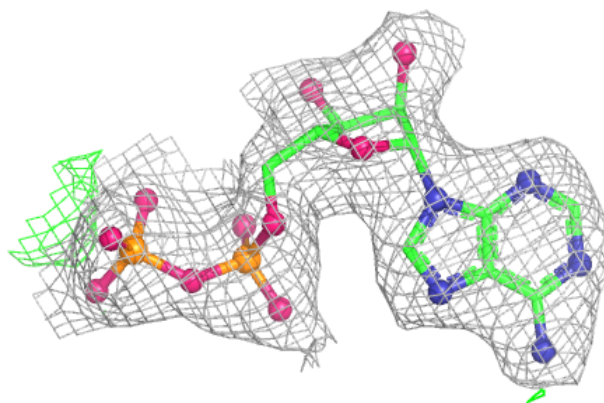
Electron density around PHY A 355:

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

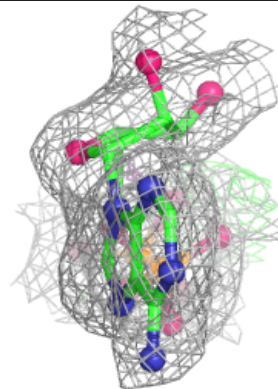
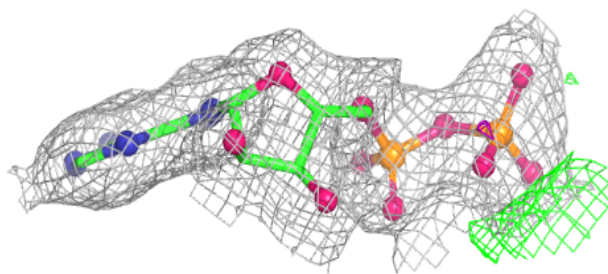
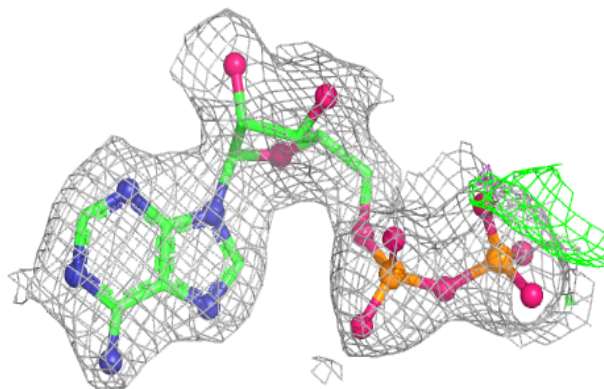


Electron density around ADP A 350:

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

**Electron density around ADP B 350:**

$2mF_o-DF_c$ (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.