



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:45 am BST

PDB ID : 1E4E
Title : D-alanyl-D-lactate 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

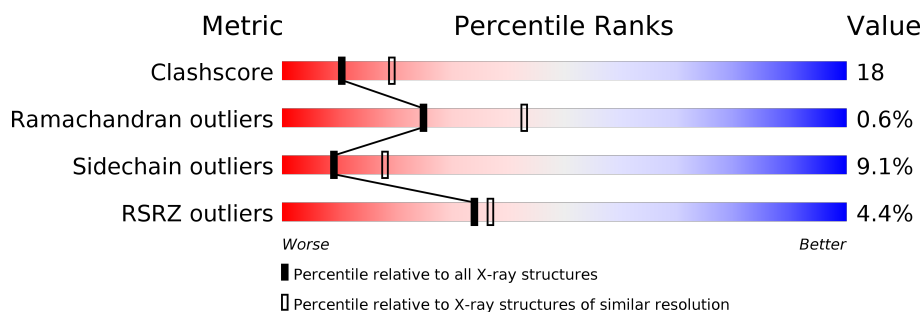
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	<div> <div>4%</div> <div>62%</div> <div>29%</div> <div>7%</div> <div>..</div> </div>
2	B	343	<div> <div>5%</div> <div>62%</div> <div>29%</div> <div>7%</div> <div>..</div> </div>

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	1347	-	-	-	X
7	GOL	A	1348	-	-	X	-
7	GOL	A	1349	-	-	-	X
7	GOL	A	1350	-	-	-	X
7	GOL	A	990	-	-	X	-
7	GOL	A	996	-	-	-	X
7	GOL	B	1346	-	-	X	-
7	GOL	B	1347	-	-	X	-
7	GOL	B	1348	-	-	-	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
1	A	341	Total	C	N	O	S	5	0	0
			2607	1653	443	496	15			

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
2	B	340	Total	C	N	O	S	33	0	0
			2603	1650	446	492	15			

There are 5 discrepancies between the modelled and reference sequences:

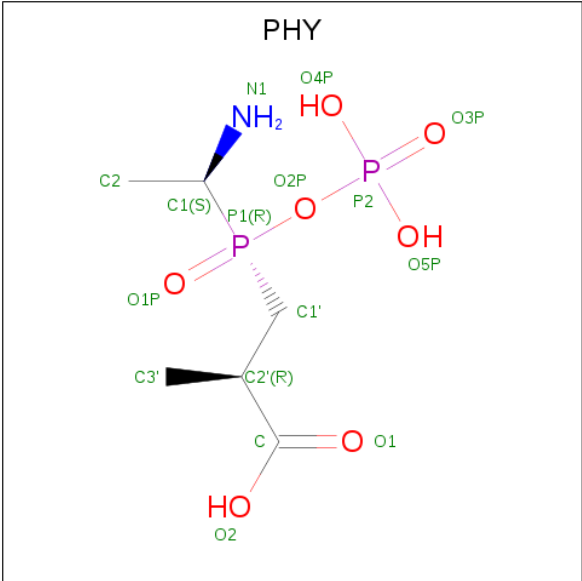
Chain	Residue	Modelled	Actual	Comment	Reference
B	62	GLU	ASP	conflict	UNP P25051
B	276	VAL	ALA	conflict	UNP P25051
B	282	THR	ALA	conflict	UNP P25051
B	298	ARG	ASN	conflict	UNP P25051
B	328	SER	ALA	conflict	UNP P25051

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (three-letter code: PHY) (formula: C₆H₁₅NO₇P₂).



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

Continued on next page...

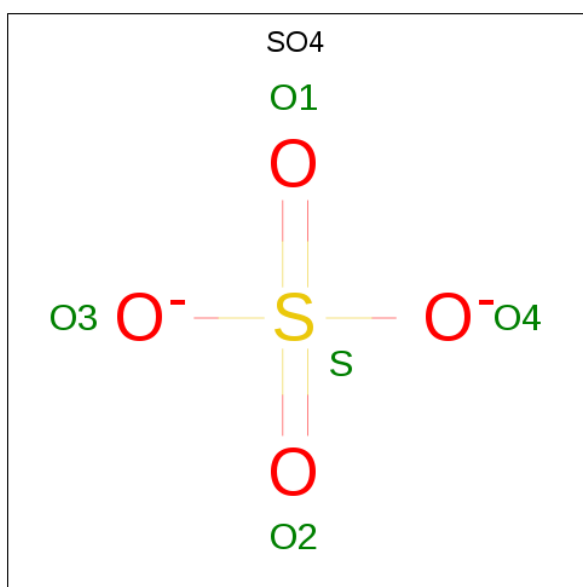
Continued from previous page...

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SULFATE ION (three-letter code: 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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

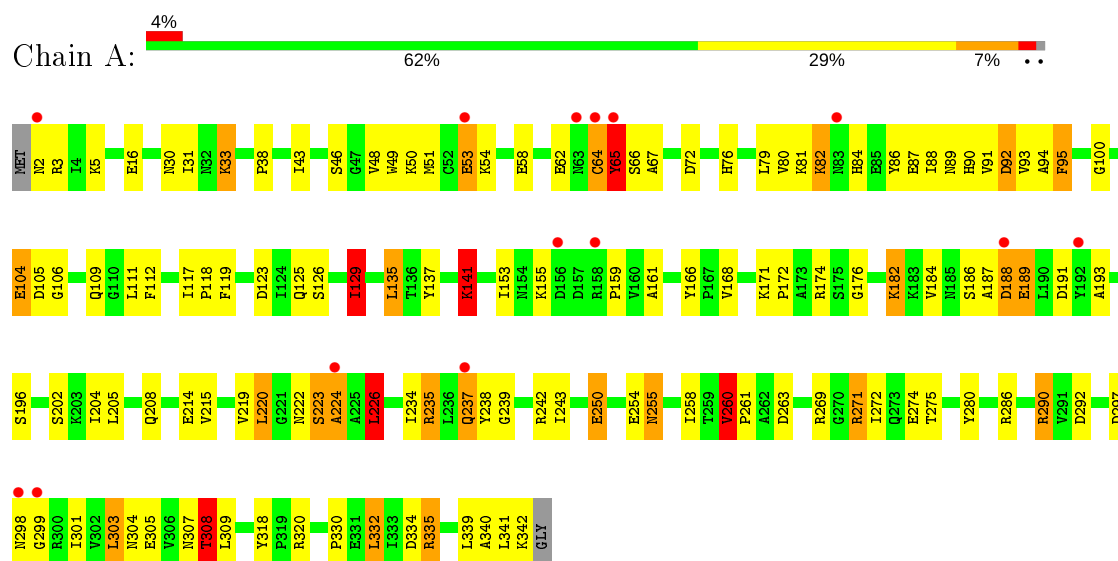
- Molecule 8 is water.

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

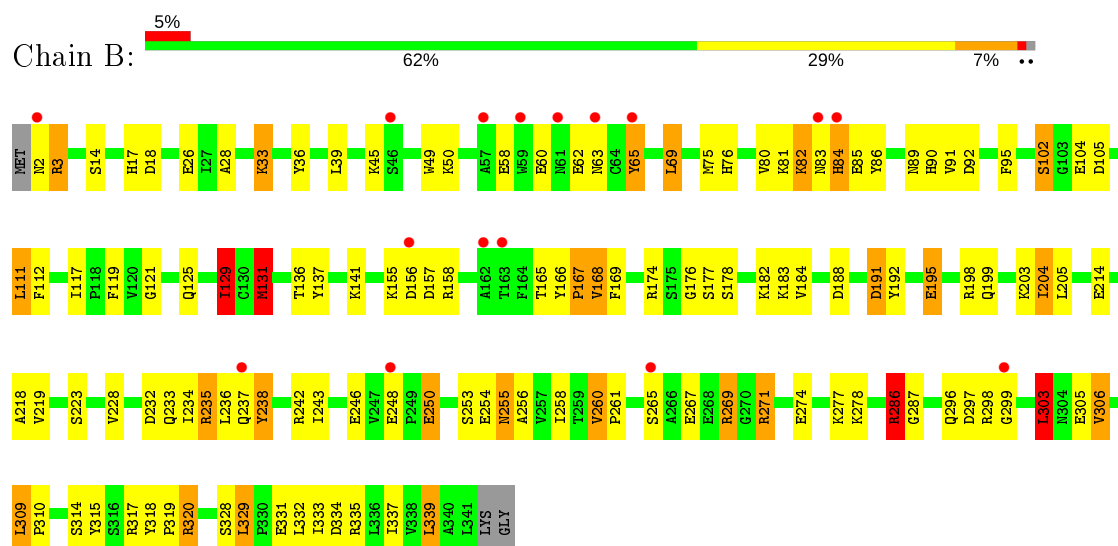
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

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 14.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.3 (15.00-2.50) 93.3 (14.86-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.88 (at 2.51Å)	Xtriage
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	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
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	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5750	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage'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: GOL, MG, PHY, ADP, SO4

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	1.41	15/2654 (0.6%)	1.52	49/3589 (1.4%)
2	B	1.51	20/2650 (0.8%)	1.61	46/3583 (1.3%)
All	All	1.46	35/5304 (0.7%)	1.57	95/7172 (1.3%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLN	CA-CB	-17.09	1.16	1.53
2	B	84	HIS	CA-CB	16.40	1.90	1.53
2	B	155	LYS	CB-CG	-15.31	1.11	1.52
2	B	62	GLU	CA-CB	-13.57	1.24	1.53
1	A	250	GLU	CD-OE1	10.83	1.37	1.25
2	B	305	GLU	CD-OE2	-9.46	1.15	1.25
2	B	306	VAL	CB-CG2	8.38	1.70	1.52
1	A	64	CYS	CB-SG	-7.45	1.69	1.82
2	B	82	LYS	CG-CD	-7.43	1.27	1.52
2	B	58	GLU	CA-CB	-7.29	1.38	1.53
2	B	183	LYS	CE-NZ	7.21	1.67	1.49
1	A	280	TYR	CE2-CZ	6.84	1.47	1.38
2	B	223	SER	CB-OG	6.77	1.51	1.42
2	B	219	VAL	CB-CG2	6.22	1.66	1.52
2	B	158	ARG	CG-CD	6.10	1.67	1.51
2	B	192	TYR	CG-CD1	-6.08	1.31	1.39
2	B	199	GLN	CG-CD	6.04	1.65	1.51
2	B	248	GLU	CD-OE1	6.04	1.32	1.25
2	B	195	GLU	CG-CD	6.02	1.60	1.51
2	B	85	GLU	CA-CB	5.98	1.67	1.53
2	B	271	ARG	CG-CD	5.96	1.66	1.51
1	A	104	GLU	CD-OE1	5.94	1.32	1.25
1	A	254	GLU	CD-OE2	5.79	1.32	1.25
1	A	93	VAL	CB-CG1	-5.68	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	235	ARG	CG-CD	5.62	1.66	1.51
2	B	191	ASP	CB-CG	-5.55	1.40	1.51
1	A	318	TYR	CE2-CZ	5.52	1.45	1.38
1	A	182	LYS	CD-CE	5.45	1.64	1.51
1	A	46	SER	CB-OG	-5.41	1.35	1.42
2	B	168	VAL	CB-CG2	-5.40	1.41	1.52
1	A	274	GLU	CD-OE1	5.22	1.31	1.25
1	A	342	LYS	CA-CB	5.18	1.65	1.53
1	A	250	GLU	CG-CD	5.18	1.59	1.51
1	A	255	ASN	CB-CG	5.09	1.62	1.51
1	A	16	GLU	CD-OE1	-5.09	1.20	1.25

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ARG	NE-CZ-NH2	-16.84	111.88	120.30
2	B	269	ARG	NE-CZ-NH1	16.51	128.55	120.30
2	B	335	ARG	NE-CZ-NH2	-16.06	112.27	120.30
2	B	84	HIS	N-CA-CB	15.70	138.87	110.60
1	A	320	ARG	NE-CZ-NH2	-13.51	113.54	120.30
2	B	271	ARG	NE-CZ-NH2	-12.19	114.21	120.30
2	B	62	GLU	CB-CA-C	12.09	134.58	110.40
2	B	3	ARG	NE-CZ-NH2	-12.05	114.27	120.30
2	B	191	ASP	CB-CG-OD2	-11.60	107.86	118.30
1	A	320	ARG	NE-CZ-NH1	10.94	125.77	120.30
2	B	271	ARG	NE-CZ-NH1	10.86	125.73	120.30
2	B	158	ARG	CB-CG-CD	10.48	138.84	111.60
2	B	235	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	A	208	GLN	N-CA-CB	9.43	127.58	110.60
2	B	320	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	208	GLN	CA-CB-CG	9.04	133.30	113.40
1	A	309	LEU	CA-CB-CG	-8.94	94.75	115.30
1	A	64	CYS	CA-CB-SG	-8.90	97.99	114.00
2	B	33	LYS	CD-CE-NZ	8.56	131.39	111.70
2	B	335	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	B	174	ARG	NE-CZ-NH2	-8.54	116.03	120.30
2	B	235	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	A	92	ASP	CB-CG-OD2	8.34	125.80	118.30
1	A	335	ARG	NE-CZ-NH1	8.21	124.41	120.30
2	B	129	ILE	CG1-CB-CG2	-7.89	94.04	111.40
2	B	174	ARG	NE-CZ-NH1	7.86	124.23	120.30
2	B	334	ASP	CB-CG-OD1	7.77	125.30	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	235	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	303	LEU	CB-CG-CD2	7.53	123.80	111.00
1	A	174	ARG	NE-CZ-NH1	-7.38	116.61	120.30
2	B	131	MET	CB-CG-SD	7.34	134.41	112.40
1	A	208	GLN	CG-CD-NE2	-7.31	99.15	116.70
2	B	286	ARG	NE-CZ-NH1	7.27	123.94	120.30
2	B	157	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	129	ILE	CG1-CB-CG2	-6.95	96.10	111.40
1	A	250	GLU	CG-CD-OE1	6.90	132.10	118.30
2	B	3	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	208	GLN	CG-CD-OE1	6.89	135.38	121.60
1	A	290	ARG	NE-CZ-NH1	-6.79	116.91	120.30
2	B	155	LYS	CA-CB-CG	6.78	128.32	113.40
1	A	65	TYR	N-CA-C	6.78	129.31	111.00
1	A	297	ASP	CB-CG-OD2	6.76	124.39	118.30
1	A	191	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	141	LYS	CA-CB-CG	6.64	128.00	113.40
1	A	135	LEU	CB-CG-CD2	-6.63	99.73	111.00
1	A	269	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	260	VAL	CB-CA-C	-6.60	98.86	111.40
2	B	62	GLU	N-CA-CB	-6.53	98.85	110.60
2	B	339	LEU	CA-CB-CG	6.52	130.29	115.30
2	B	320	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	B	305	GLU	OE1-CD-OE2	-6.32	115.71	123.30
2	B	18	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	105	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	335	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	B	303	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	235	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	342	LYS	N-CA-C	6.13	127.56	111.00
1	A	286	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	263	ASP	CB-CG-OD1	5.89	123.60	118.30
2	B	3	ARG	CD-NE-CZ	5.88	131.83	123.60
2	B	260	VAL	CB-CA-C	-5.86	100.27	111.40
1	A	298	ASN	N-CA-CB	-5.77	100.21	110.60
1	A	242	ARG	NE-CZ-NH1	-5.75	117.42	120.30
2	B	238	TYR	CB-CG-CD1	5.74	124.44	121.00
1	A	208	GLN	CB-CA-C	5.72	121.85	110.40
2	B	297	ASP	CB-CG-OD1	5.70	123.43	118.30
2	B	105	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	182	LYS	CD-CE-NZ	5.54	124.45	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	CYS	N-CA-CB	-5.52	100.66	110.60
2	B	191	ASP	CB-CG-OD1	5.50	123.25	118.30
2	B	111	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	72	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	341	LEU	O-C-N	-5.45	113.98	122.70
2	B	156	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	208	GLN	CB-CG-CD	5.43	125.71	111.60
1	A	308	THR	N-CA-CB	-5.40	100.03	110.30
2	B	92	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	332	LEU	CB-CG-CD1	-5.37	101.86	111.00
1	A	334	ASP	CB-CG-OD1	5.37	123.14	118.30
2	B	317	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	64	CYS	CA-C-N	5.26	128.77	117.20
1	A	271	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	243	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	A	303	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	271	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	B	167	PRO	N-CD-CG	-5.12	95.52	103.20
2	B	81	LYS	CB-CG-CD	5.11	124.89	111.60
2	B	310	PRO	N-CD-CG	-5.10	95.55	103.20
1	A	64	CYS	N-CA-C	5.10	124.77	111.00
2	B	158	ARG	CG-CD-NE	5.05	122.40	111.80
1	A	340	ALA	CA-C-O	5.04	130.68	120.10
2	B	232	ASP	CB-CG-OD2	5.04	122.83	118.30
2	B	235	ARG	CD-NE-CZ	5.01	130.61	123.60
1	A	141	LYS	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2607	0	2602	100	4
2	B	2603	0	2607	85	0
3	A	27	0	12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	12	0
8	A	175	0	0	6	0
8	B	180	0	0	17	0
All	All	5750	0	5353	197	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 18.

All (197) 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
4:B:355:PHY:C2	4:B:355:PHY:P1	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	0.83
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1344:SO4:S	8:B:3009:HOH:O	2.42	0.77
1:A:271:ARG:NH2	1:A:299:GLY:O	2.19	0.76
2:B:265:SER:HB2	8:B:2137:HOH:O	1.86	0.75
2:B:83:ASN:CG	2:B:84:HIS:H	1.92	0.73
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
2:B:250:GLU:H	2:B:250:GLU:CD	1.95	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:H	2:B:255:ASN:HD22	1.42	0.68
2:B:168:VAL:O	2:B:184:VAL:N	2.22	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: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
2:B:296:GLN:O	2:B:299:GLY:N	2.33	0.60
4:B:355:PHY:O3P	4:B:355:PHY:H1'2	2.01	0.60
1:A:51:MET:HE2	1:A:65:TYR:CE2	2.37	0.59
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
1:A:51:MET:CE	1:A:65:TYR:CE2	2.87	0.58
2:B:314:SER:HA	7:B:1347:GOL:C3	2.24	0.58
1:A:88:ILE:C	1:A:89:ASN:HD22	2.08	0.57
1:A:215:VAL:HG21	1:A:272:ILE:HD13	1.85	0.57
1:A:51:MET:CE	1:A:65:TYR:CD2	2.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:51:MET:HE2	1:A:65:TYR:CD2	2.42	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
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: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:218:ALA:HB1	2:B:318:TYR:CE2	2.45	0.52
2:B:36:TYR:CE1	2:B:337:ILE:HG21	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
1:A:31:ILE:HG23	1:A:33:LYS:HE3	1.92	0.51
1:A:95:PHE:C	1:A:95:PHE:CD1	2.83	0.51
2:B:83:ASN:CG	2:B:84:HIS:N	2.62	0.51
2:B:233:GLN:O	2:B:258:ILE:HA	2.11	0.51
1:A:51:MET:HE1	1:A:65:TYR:CD2	2.46	0.51
2:B:203:LYS:HE2	6:B:1342:SO4:O4	2.11	0.51
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:100:GLY:N	1:A:104:GLU:OE1	2.39	0.50
1:A:89:ASN:N	1:A:89:ASN:ND2	2.59	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:N	1:A:89:ASN:HD22	2.10	0.50
1:A:43:ILE:HA	1:A:48:VAL:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:HIS:CD2	1:A:91:VAL:O	2.65	0.49
2:B:75:MET:O	2:B:76:HIS:C	2.49	0.49
2:B:166:TYR:HB3	2:B:167:PRO:HA	1.95	0.49
1:A:125:GLN:O	1:A:129:ILE:HG12	2.13	0.49
1:A:260:VAL:HA	1:A:261:PRO:C	2.31	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:HD2	2:B:76:HIS:O	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
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:N	1:A:188:ASP:OD1	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:121:GLY:HA2	2:B:287:GLY:HA3	1.97	0.46
2:B:204:ILE:HD12	2:B:204:ILE:C	2.36	0.46
2:B:129:ILE:HD12	2:B:129:ILE:HG21	1.49	0.46
1:A:214:GLU:OE2	3:A:350:ADP:O2'	2.26	0.46
1:A:222:ASN:O	1:A:223:SER:C	2.54	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:274:GLU:O	2:B:278:LYS:HG2	2.16	0.45
1:A:95:PHE:C	1:A:95:PHE:HD1	2.20	0.45
2:B:90:HIS:ND1	8:B:2048:HOH:O	2.36	0.45
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.83	0.45
2:B:318:TYR:N	2:B:319:PRO:CD	2.80	0.45
1:A:51:MET:O	1:A:64:CYS:C	2.48	0.44
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:219:VAL:HG12	1:A:220:LEU:N	2.32	0.44
1:A:51:MET:HB3	1:A:65:TYR:CG	2.53	0.44
1:A:76:HIS:HD2	1:A:76:HIS:O	2.00	0.44
2:B:76:HIS:CD2	2:B:91:VAL:O	2.71	0.44
1:A:65:TYR:O	1:A:66:SER:C	2.54	0.44
1:A:62:GLU:OE1	1:A:62:GLU:HA	2.17	0.44
1:A:51:MET:C	1:A:65:TYR:H	1.98	0.44
1:A:129:ILE:HG22	1:A:135:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:SER:HA	1:A:129:ILE:HG12	2.00	0.43
1:A:3:ARG:HG3	7:A:1348:GOL:C1	2.45	0.43
2:B:234:ILE:HG12	2:B:258:ILE:HG12	1.99	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:204:ILE:HD12	1:A:204:ILE:C	2.38	0.43
1:A:49:TRP:HB3	1:A:67:ALA:O	2.19	0.43
2:B:112:PHE:HB3	2:B:119:PHE:CD1	2.54	0.43
2:B:3:ARG:CD	2:B:33:LYS:O	2.67	0.43
1:A:226:LEU:CD1	1:A:226:LEU:N	2.82	0.43
1:A:104:GLU:HG2	1:A:308:THR:HG22	2.01	0.42
1:A:226:LEU:H	1:A:226:LEU:CD1	2.32	0.42
1:A:176:GLY:HA2	3:A:350:ADP:O1B	2.19	0.42
2:B:236:LEU:HD23	2:B:256:ALA:CB	2.48	0.42
2:B:309:LEU:HA	2:B:309:LEU:HD22	1.94	0.42
2:B:129:ILE:HD13	2:B:129:ILE:HG23	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
2:B:242:ARG:O	2:B:243:ILE:C	2.57	0.42
1:A:51:MET:O	1:A:64:CYS:HA	2.20	0.41
2:B:269:ARG:HD2	8:B:2141:HOH:O	2.20	0.41
2:B:80:VAL:O	2:B:86:TYR:HA	2.20	0.41
2:B:246:GLU:OE1	2:B:254:GLU:N	2.40	0.41
2:B:28:ALA:O	2:B:33:LYS:NZ	2.45	0.41
2:B:315:TYR:O	2:B:320:ARG:NH1	2.53	0.41
2:B:250:GLU:N	2:B:250:GLU:CD	2.68	0.41
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:260:VAL:HA	2:B:261:PRO:C	2.41	0.41
2:B:39:LEU:CD1	7:B:1346:GOL:H31	2.50	0.41
1:A:129:ILE:HG21	1:A:129:ILE:HD12	1.54	0.41
1:A:290:ARG:HD3	1:A:290:ARG:HH11	1.62	0.41
1:A:214:GLU:OE2	3:A:350:ADP:H2'	2.21	0.41
1:A:65:TYR:N	1:A:65:TYR:HD1	2.18	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:166:TYR:CZ	1:A:187:ALA:HA	2.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:SER:O	2:B:178:SER:HB2	2.21	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
1:A:307:ASN:HB3	8:A:2154:HOH:O	2.21	0.40
1:A:117:ILE:HG22	1:A:118:PRO:O	2.22	0.40
1:A:30:ASN:HB3	1:A:330:PRO:HG3	2.03	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%)	17	31
2	B	338/343 (98%)	322 (95%)	15 (4%)	1 (0%)	41	61
All	All	677/686 (99%)	641 (95%)	32 (5%)	4 (1%)	25	43

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 ⓘ

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%)	254 (91%)	25 (9%)	9	19
2	B	279/285 (98%)	253 (91%)	26 (9%)	9	17
All	All	558/570 (98%)	507 (91%)	51 (9%)	9	18

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	53	GLU
1	A	65	TYR
1	A	82	LYS
1	A	95	PHE
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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	260	VAL
1	A	303	LEU
1	A	305	GLU
1	A	308	THR
1	A	332	LEU
2	B	63	ASN
2	B	65	TYR
2	B	69	LEU
2	B	82	LYS
2	B	95	PHE
2	B	102	SER
2	B	111	LEU
2	B	129	ILE
2	B	131	MET
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	250	GLU
2	B	255	ASN
2	B	267	GLU
2	B	286	ARG
2	B	298	ARG
2	B	303	LEU
2	B	309	LEU
2	B	329	LEU
2	B	331	GLU
2	B	332	LEU
2	B	339	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	255	ASN
2	B	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	76	HIS
2	B	125	GLN
2	B	154	ASN
2	B	255	ASN
2	B	304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
7	GOL	B	1344	-	5,5,5	0.35	0	5,5,5	0.30	0
6	SO4	B	1342	-	4,4,4	0.41	0	6,6,6	0.87	0
6	SO4	A	1344	-	4,4,4	0.29	0	6,6,6	0.42	0
4	PHY	A	355	5	2,11,15	1.05	0	0,14,23	0.00	-
7	GOL	A	1349	-	5,5,5	0.48	0	5,5,5	0.36	0
7	GOL	B	1347	-	5,5,5	0.62	0	5,5,5	1.03	1 (20%)
7	GOL	A	1347	-	5,5,5	0.61	0	5,5,5	0.81	0
3	ADP	A	350	5	24,29,29	1.53	5 (20%)	29,45,45	1.48	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	350	5	24,29,29	1.51	3 (12%)	29,45,45	1.47	4 (13%)
7	GOL	B	1343	-	5,5,5	0.30	0	5,5,5	1.43	1 (20%)
7	GOL	A	1350	-	5,5,5	0.45	0	5,5,5	0.37	0
7	GOL	A	990	-	5,5,5	0.50	0	5,5,5	1.75	1 (20%)
7	GOL	A	996	-	5,5,5	0.55	0	5,5,5	0.49	0
7	GOL	B	1345	-	5,5,5	0.37	0	5,5,5	1.93	2 (40%)
6	SO4	A	1343	-	4,4,4	0.12	0	6,6,6	1.35	1 (16%)
4	PHY	B	355	5	2,11,15	0.53	0	0,14,23	0.00	-
7	GOL	B	1346	-	5,5,5	0.41	0	5,5,5	0.48	0
7	GOL	A	1345	-	5,5,5	1.56	1 (20%)	5,5,5	2.92	3 (60%)
7	GOL	A	1348	-	5,5,5	0.52	0	5,5,5	2.14	3 (60%)
7	GOL	B	1348	-	5,5,5	0.43	0	5,5,5	0.56	0
7	GOL	A	1346	-	5,5,5	1.00	0	5,5,5	2.15	2 (40%)

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
7	GOL	B	1344	-	-	2/4/4/4	-
7	GOL	A	990	-	-	1/4/4/4	-
4	PHY	A	355	5	-	1/1/12/21	-
7	GOL	A	1349	-	-	2/4/4/4	-
7	GOL	B	1347	-	-	2/4/4/4	-
7	GOL	A	1347	-	-	4/4/4/4	-
3	ADP	A	350	5	-	4/12/32/32	0/3/3/3
3	ADP	B	350	5	-	8/12/32/32	0/3/3/3
7	GOL	B	1343	-	-	2/4/4/4	-
7	GOL	A	1350	-	-	2/4/4/4	-
7	GOL	B	1346	-	-	4/4/4/4	-
7	GOL	A	996	-	-	4/4/4/4	-
7	GOL	B	1345	-	-	3/4/4/4	-
4	PHY	B	355	5	-	0/1/12/21	-
7	GOL	A	1345	-	-	3/4/4/4	-
7	GOL	A	1348	-	-	1/4/4/4	-
7	GOL	B	1348	-	-	4/4/4/4	-
7	GOL	A	1346	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	350	ADP	C2-N3	4.50	1.39	1.32
3	A	350	ADP	O4'-C1'	4.10	1.46	1.41
3	A	350	ADP	C2-N1	3.00	1.39	1.33
7	A	1345	GOL	O2-C2	-2.76	1.35	1.43
3	B	350	ADP	C2-N1	2.73	1.39	1.33
3	A	350	ADP	PB-O3B	-2.58	1.44	1.54
3	B	350	ADP	C3'-C4'	-2.58	1.46	1.53
3	A	350	ADP	O3'-C3'	-2.39	1.37	1.43
3	A	350	ADP	C2-N3	2.09	1.35	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1345	GOL	O2-C2-C3	-4.51	89.25	109.12
3	A	350	ADP	N3-C2-N1	-4.15	122.20	128.68
7	A	1345	GOL	C3-C2-C1	-4.04	95.98	111.70
3	B	350	ADP	N3-C2-N1	-3.98	122.45	128.68
3	B	350	ADP	O5'-C5'-C4'	3.25	120.17	108.99
3	A	350	ADP	O3B-PB-O3A	3.24	115.50	104.64
7	A	1346	GOL	O2-C2-C3	-3.18	95.12	109.12
7	A	1346	GOL	O3-C3-C2	-3.09	95.40	110.20
3	B	350	ADP	O3B-PB-O2B	2.88	118.64	107.64
7	A	1348	GOL	C3-C2-C1	2.76	122.45	111.70
7	B	1345	GOL	O2-C2-C1	2.67	120.89	109.12
7	A	1348	GOL	O2-C2-C3	2.59	120.54	109.12
7	B	1345	GOL	O3-C3-C2	-2.51	98.19	110.20
7	B	1343	GOL	O2-C2-C3	2.44	119.85	109.12
7	A	1345	GOL	O2-C2-C1	-2.34	98.82	109.12
3	A	350	ADP	C3'-C2'-C1'	-2.31	97.50	100.98
3	B	350	ADP	C5'-C4'-C3'	-2.29	106.59	115.18
6	A	1343	SO4	O3-S-O1	-2.23	97.66	109.31
7	A	1348	GOL	O3-C3-C2	2.21	120.78	110.20
7	A	990	GOL	O3-C3-C2	2.17	120.61	110.20
3	A	350	ADP	O3B-PB-O2B	2.15	115.84	107.64
7	B	1347	GOL	O3-C3-C2	2.13	120.43	110.20

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1346	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	350	ADP	PA-O3A-PB-O2B
7	B	1346	GOL	C1-C2-C3-O3
3	B	350	ADP	PA-O3A-PB-O2B
3	B	350	ADP	PA-O3A-PB-O3B
4	A	355	PHY	P1-C1'-C2'-C3'
7	B	1345	GOL	C1-C2-C3-O3
7	B	1345	GOL	O2-C2-C3-O3
7	B	1348	GOL	O1-C1-C2-C3
7	B	1348	GOL	C1-C2-C3-O3
7	A	1349	GOL	O1-C1-C2-C3
7	B	1347	GOL	O1-C1-C2-C3
7	B	1343	GOL	C1-C2-C3-O3
7	A	996	GOL	C1-C2-C3-O3
7	A	1345	GOL	O2-C2-C3-O3
7	A	1346	GOL	C1-C2-C3-O3
7	B	1344	GOL	O1-C1-C2-C3
7	B	1346	GOL	O1-C1-C2-C3
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	B	1345	GOL	O1-C1-C2-C3
7	A	1345	GOL	O1-C1-C2-C3
7	A	1345	GOL	C1-C2-C3-O3
7	A	996	GOL	O1-C1-C2-C3
7	B	1346	GOL	O1-C1-C2-O2
7	A	1347	GOL	O1-C1-C2-O2
7	B	1348	GOL	O1-C1-C2-O2
7	A	1349	GOL	O1-C1-C2-O2
7	B	1347	GOL	O1-C1-C2-O2
7	B	1343	GOL	O2-C2-C3-O3
7	A	996	GOL	O1-C1-C2-O2
7	A	1346	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	996	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
3	A	350	ADP	C4'-C5'-O5'-PA
3	B	350	ADP	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

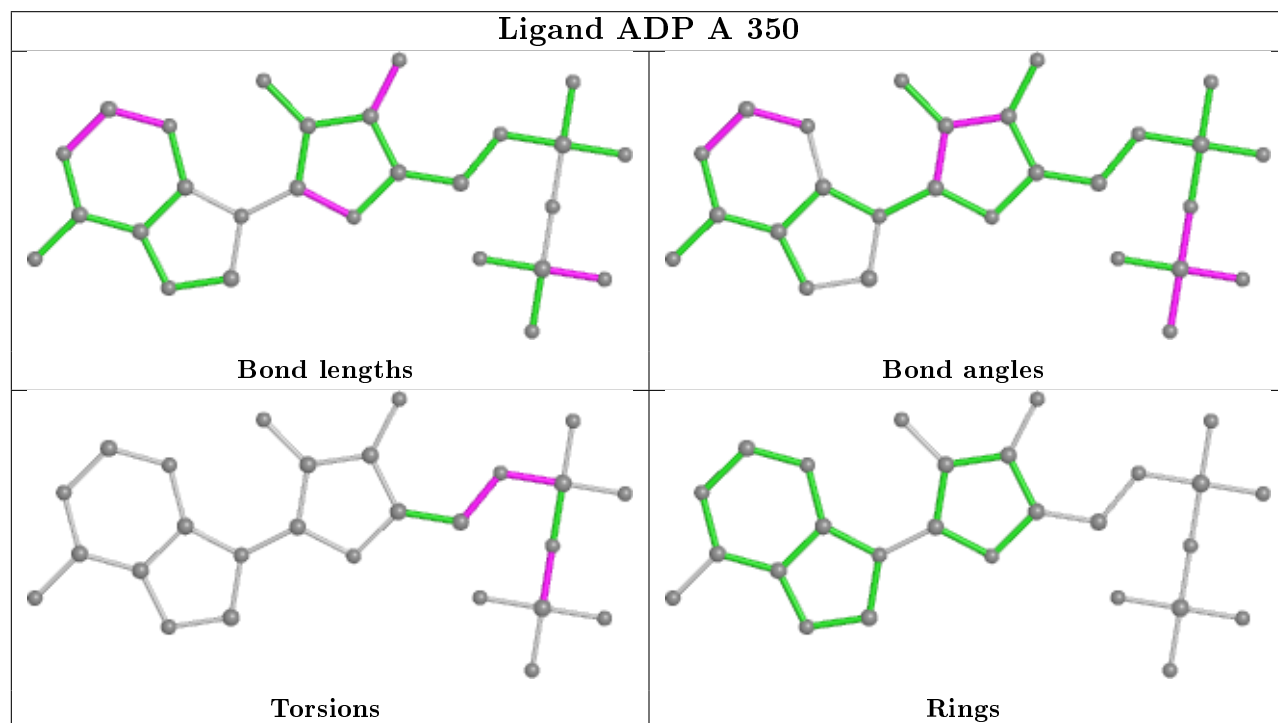
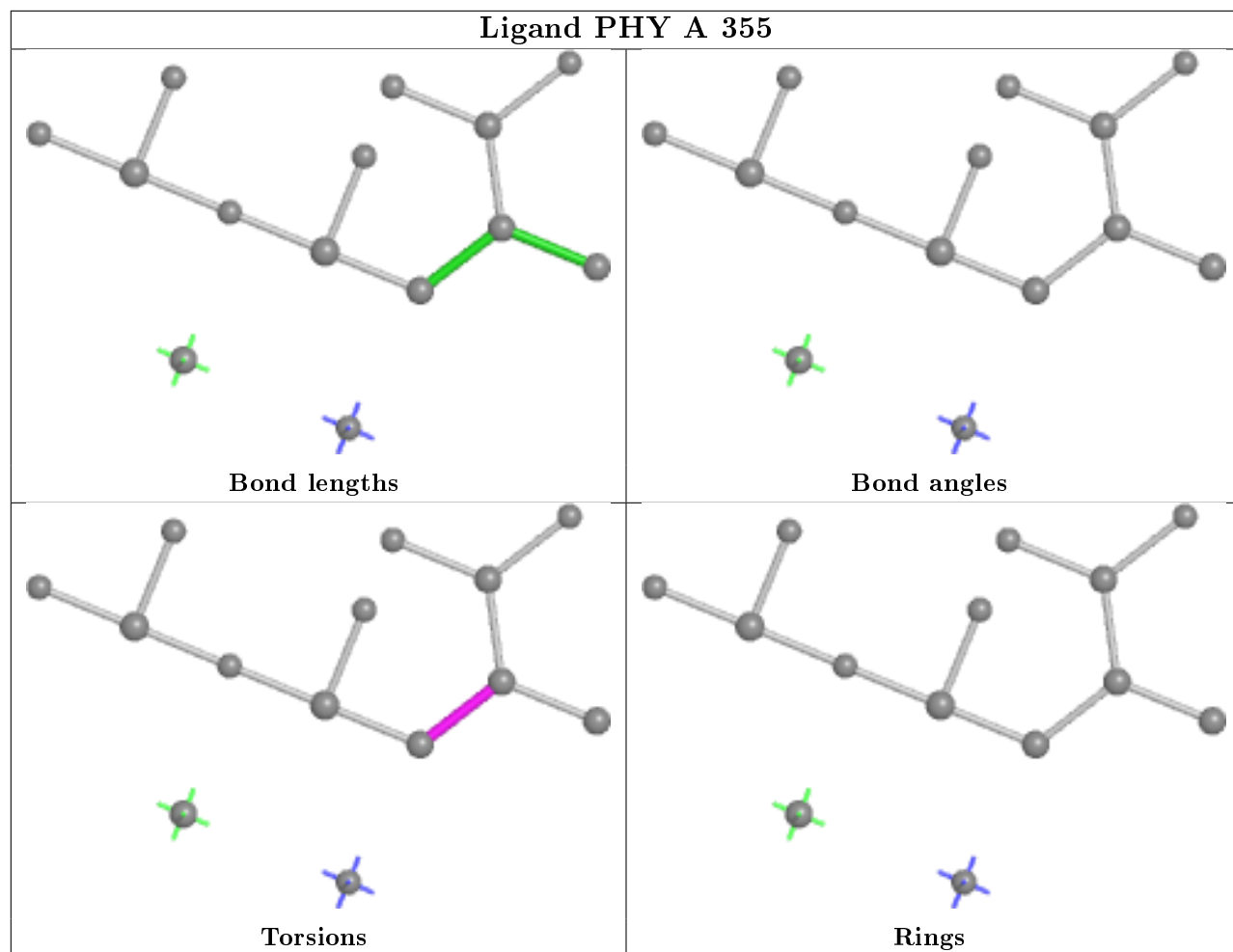
Mol	Chain	Res	Type	Atoms
3	B	350	ADP	PB-O3A-PA-O2A
7	A	1348	GOL	O2-C2-C3-O3
3	B	350	ADP	C3'-C4'-C5'-O5'
3	A	350	ADP	PA-O3A-PB-O3B
3	A	350	ADP	C5'-O5'-PA-O3A
3	B	350	ADP	C5'-O5'-PA-O3A
3	B	350	ADP	C5'-O5'-PA-O1A
7	A	990	GOL	O2-C2-C3-O3

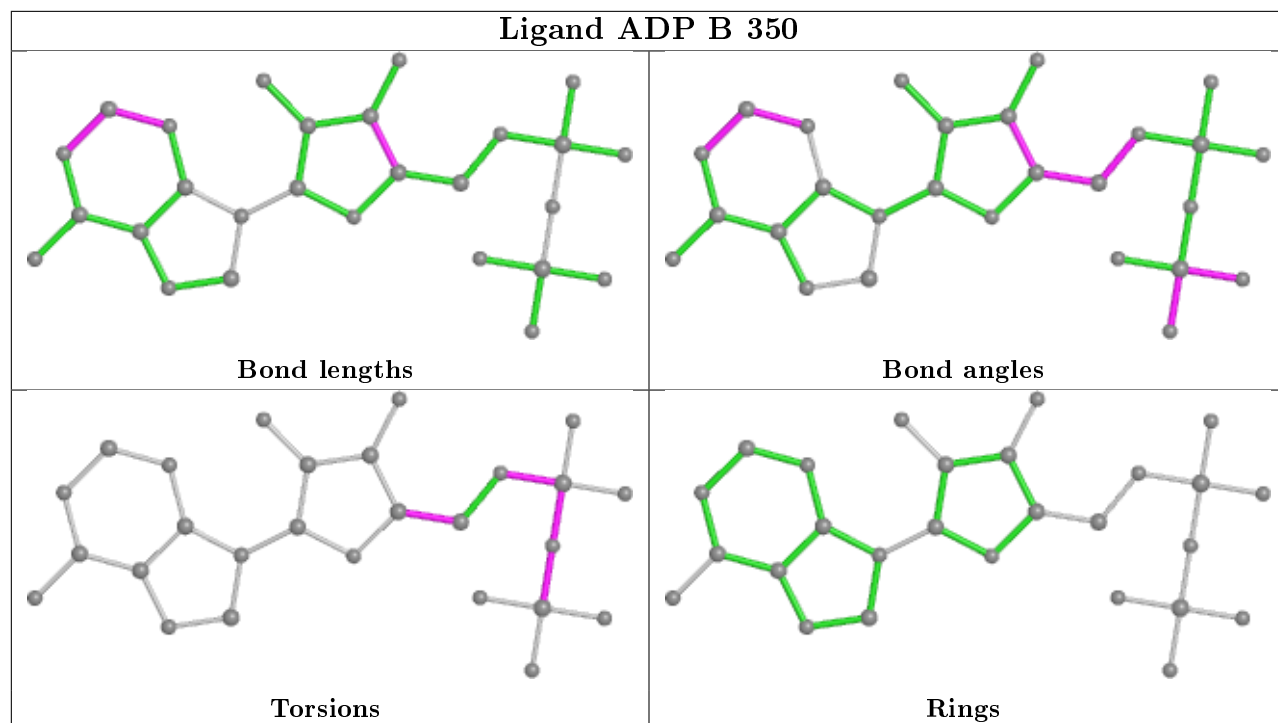
There are no ring outliers.

14 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1342	SO4	1	0
6	A	1344	SO4	4	0
4	A	355	PHY	4	0
7	B	1347	GOL	5	0
7	A	1347	GOL	2	0
3	A	350	ADP	3	0
3	B	350	ADP	2	0
7	A	1350	GOL	1	0
7	A	990	GOL	0	4
4	B	355	PHY	4	0
7	B	1346	GOL	5	0
7	A	1348	GOL	4	0
7	B	1348	GOL	2	0
7	A	1346	GOL	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/343 (99%)	-0.01	14 (4%) 37 40	41, 52, 72, 88	1 (0%)
2	B	340/343 (99%)	0.07	16 (4%) 31 33	39, 50, 72, 86	8 (2%)
All	All	681/686 (99%)	0.03	30 (4%) 34 37	39, 51, 72, 88	9 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	TYR	6.7
2	B	83	ASN	4.6
1	A	63	ASN	4.4
2	B	84	HIS	4.0
2	B	63	ASN	3.6
2	B	163	THR	3.5
2	B	162	ALA	3.3
1	A	192	TYR	3.2
2	B	156	ASP	2.9
2	B	248	GLU	2.7
2	B	59	TRP	2.7
2	B	2	ASN	2.6
2	B	237	GLN	2.6
1	A	156	ASP	2.6
1	A	224	ALA	2.5
2	B	57	ALA	2.5
1	A	188	ASP	2.5
2	B	299	GLY	2.5
1	A	299	GLY	2.5
1	A	2	ASN	2.4
1	A	64	CYS	2.4
2	B	265	SER	2.4
2	B	61	ASN	2.3
2	B	65	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	83	ASN	2.2
2	B	46	SER	2.2
1	A	53	GLU	2.1
1	A	298	ASN	2.1
1	A	237	GLN	2.1
1	A	158	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
7	GOL	B	1348	6/6	0.47	0.59	92,94,94,94	0
7	GOL	A	1349	6/6	0.47	0.60	106,108,109,109	0
7	GOL	A	1350	6/6	0.56	0.49	125,126,126,127	0
7	GOL	A	996	6/6	0.56	0.46	116,117,118,119	0
7	GOL	B	1346	6/6	0.65	0.38	95,100,101,103	0
7	GOL	A	1347	6/6	0.71	0.45	61,67,74,80	0
7	GOL	B	1343	6/6	0.73	0.31	99,101,102,103	0
7	GOL	B	1345	6/6	0.73	0.29	68,72,73,74	0
7	GOL	A	990	6/6	0.79	0.25	73,80,85,92	0
7	GOL	B	1344	6/6	0.86	0.40	104,107,108,112	0
7	GOL	B	1347	6/6	0.86	0.40	82,84,87,88	0
7	GOL	A	1348	6/6	0.87	0.31	83,84,85,87	0
5	MG	A	360	1/1	0.91	0.12	46,46,46,46	0
5	MG	B	360	1/1	0.92	0.11	42,42,42,42	0
7	GOL	A	1345	6/6	0.94	0.20	47,57,62,66	0
4	PHY	A	355	14/16	0.94	0.14	34,40,42,44	0
7	GOL	A	1346	6/6	0.95	0.18	71,72,73,73	0

Continued on next page...

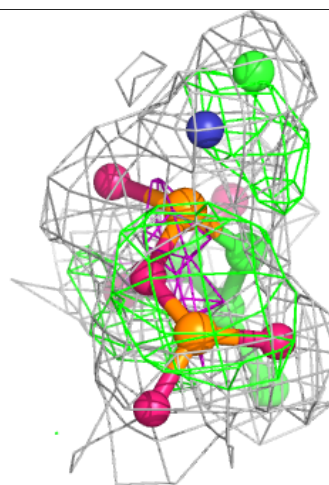
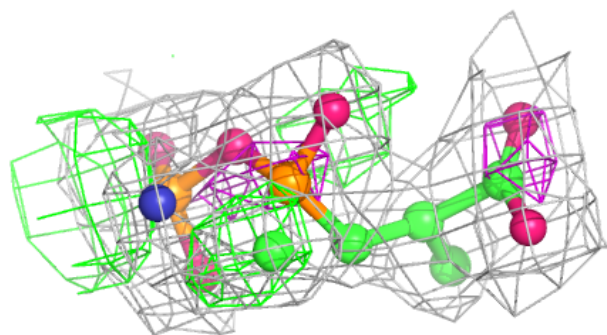
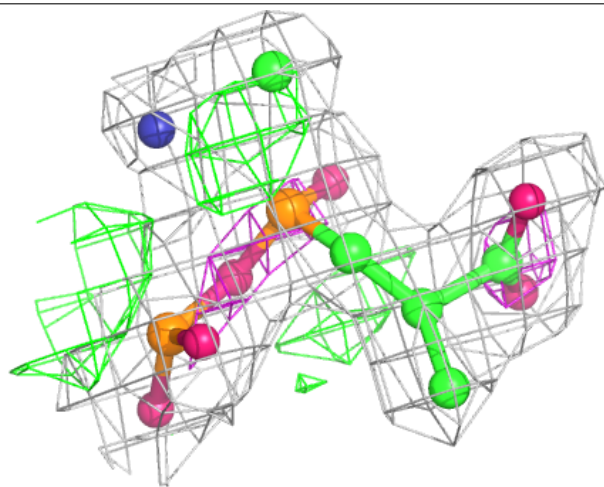
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PHY	B	355	14/16	0.96	0.14	33,35,39,39	0
3	ADP	B	350	27/27	0.96	0.12	33,45,50,51	0
6	SO4	A	1344	5/5	0.96	0.27	93,96,98,98	0
6	SO4	B	1342	5/5	0.97	0.20	50,54,56,57	0
3	ADP	A	350	27/27	0.97	0.11	41,47,51,52	0
5	MG	A	365	1/1	0.97	0.06	42,42,42,42	0
6	SO4	A	1343	5/5	0.97	0.26	56,59,62,65	0
5	MG	B	365	1/1	0.98	0.08	38,38,38,38	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.

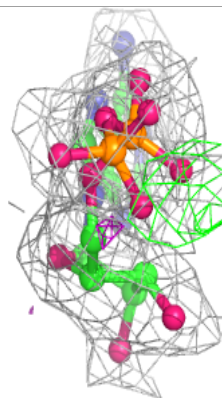
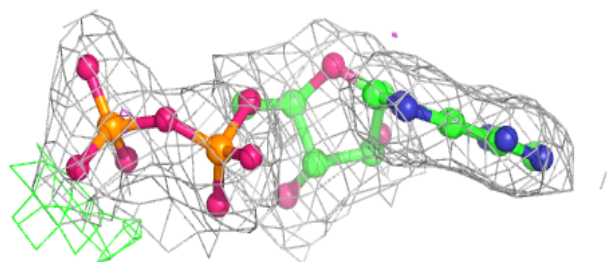
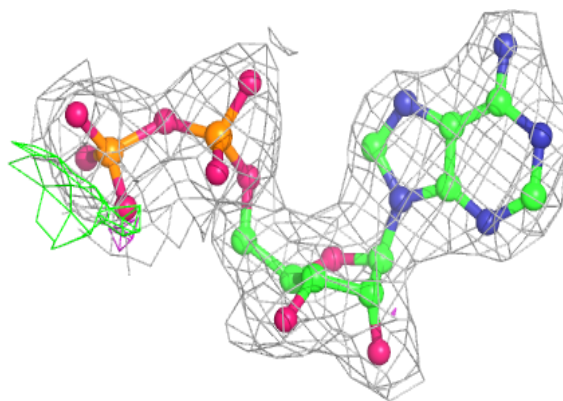
Electron density around PHY A 355:

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

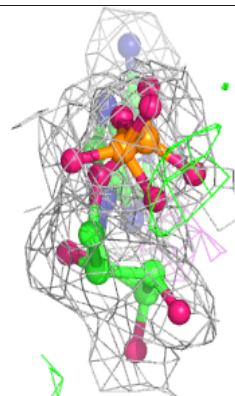
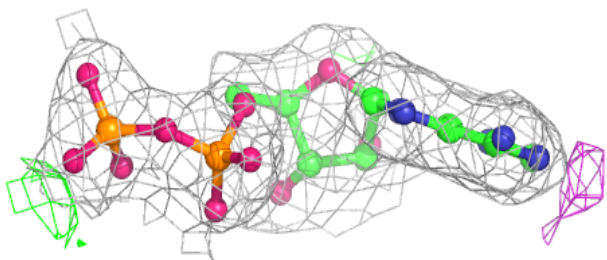
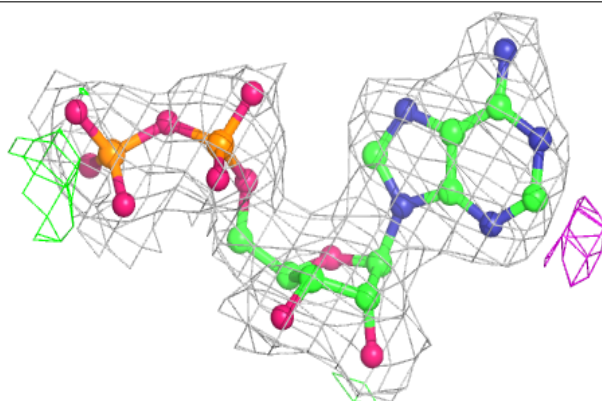


Electron density around ADP B 350:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.