



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 9IGR / pdb_00009igr
Title : Crystal structure of PPK2 class III from Erysipelotrichaceae bacterium in complex with polyphosphate
Authors : Rasche, R.; Lawrence-Doerner, A.-M.; Cornelissen, N.V.; Kuemmel, D.
Deposited on : 2025-02-20
Resolution : 2.31 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

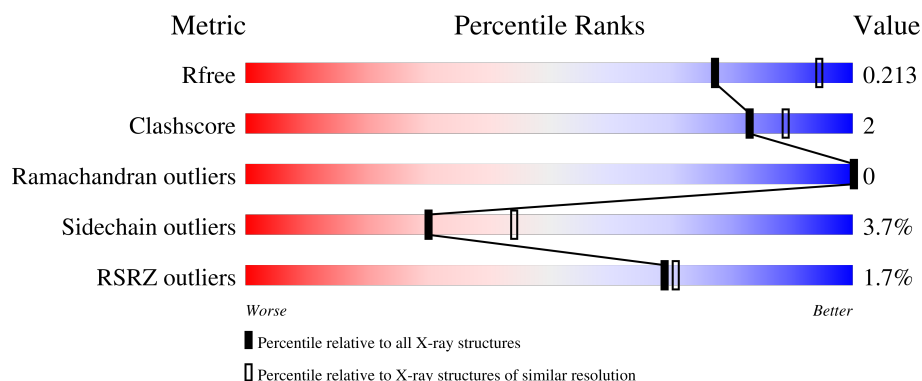
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	306	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	306	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>• •</div> </div> </div>
1	C	306	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>• •</div> </div> </div>
1	D	306	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>14%</div> <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
4	PO4	D	402	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20072 atoms, of which 9633 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 Polyphosphate--nucleotide phosphotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	H	N	O	S	0	0	0
			4798	1566	2347	410	470	5			
1	B	301	Total	C	H	N	O	S	0	0	0
			4968	1620	2431	428	484	5			
1	C	302	Total	C	H	N	O	S	0	0	0
			4984	1626	2437	431	485	5			
1	D	297	Total	C	H	N	O	S	0	0	0
			4911	1600	2408	420	478	5			

There are 36 discrepancies between the modelled and reference sequences:

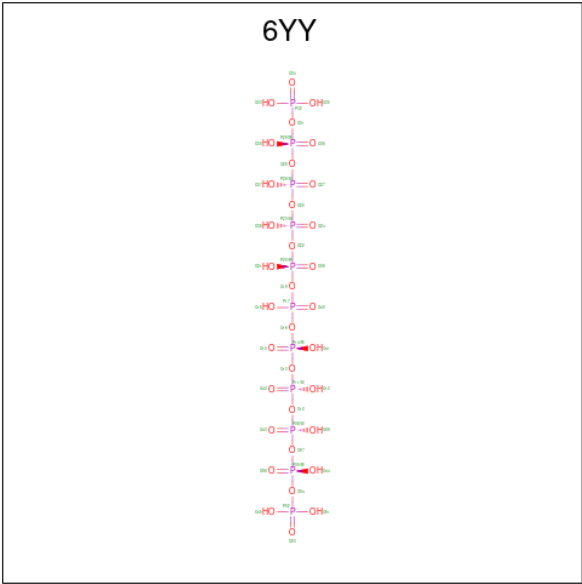
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	ILE	engineered mutation	UNP A0A3D5XRJ5
A	299	LEU	-	expression tag	UNP A0A3D5XRJ5
A	300	GLU	-	expression tag	UNP A0A3D5XRJ5
A	301	HIS	-	expression tag	UNP A0A3D5XRJ5
A	302	HIS	-	expression tag	UNP A0A3D5XRJ5
A	303	HIS	-	expression tag	UNP A0A3D5XRJ5
A	304	HIS	-	expression tag	UNP A0A3D5XRJ5
A	305	HIS	-	expression tag	UNP A0A3D5XRJ5
A	306	HIS	-	expression tag	UNP A0A3D5XRJ5
B	2	ALA	ILE	engineered mutation	UNP A0A3D5XRJ5
B	299	LEU	-	expression tag	UNP A0A3D5XRJ5
B	300	GLU	-	expression tag	UNP A0A3D5XRJ5
B	301	HIS	-	expression tag	UNP A0A3D5XRJ5
B	302	HIS	-	expression tag	UNP A0A3D5XRJ5
B	303	HIS	-	expression tag	UNP A0A3D5XRJ5
B	304	HIS	-	expression tag	UNP A0A3D5XRJ5
B	305	HIS	-	expression tag	UNP A0A3D5XRJ5
B	306	HIS	-	expression tag	UNP A0A3D5XRJ5
C	2	ALA	ILE	engineered mutation	UNP A0A3D5XRJ5
C	299	LEU	-	expression tag	UNP A0A3D5XRJ5
C	300	GLU	-	expression tag	UNP A0A3D5XRJ5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	301	HIS	-	expression tag	UNP A0A3D5XRJ5
C	302	HIS	-	expression tag	UNP A0A3D5XRJ5
C	303	HIS	-	expression tag	UNP A0A3D5XRJ5
C	304	HIS	-	expression tag	UNP A0A3D5XRJ5
C	305	HIS	-	expression tag	UNP A0A3D5XRJ5
C	306	HIS	-	expression tag	UNP A0A3D5XRJ5
D	2	ALA	ILE	engineered mutation	UNP A0A3D5XRJ5
D	299	LEU	-	expression tag	UNP A0A3D5XRJ5
D	300	GLU	-	expression tag	UNP A0A3D5XRJ5
D	301	HIS	-	expression tag	UNP A0A3D5XRJ5
D	302	HIS	-	expression tag	UNP A0A3D5XRJ5
D	303	HIS	-	expression tag	UNP A0A3D5XRJ5
D	304	HIS	-	expression tag	UNP A0A3D5XRJ5
D	305	HIS	-	expression tag	UNP A0A3D5XRJ5
D	306	HIS	-	expression tag	UNP A0A3D5XRJ5

- Molecule 2 is bis[oxidanyl-[oxidanyl-[oxidanyl-[oxidanyl(phosphonooxy)phosphoryl]oxy-phosphoryl]oxy-phosphoryl]oxy-phosphoryl] hydrogen phosphate (CCD ID: 6YY) (formula: H₁₃O₃₄P₁₁) (labeled as "Ligand of Interest" by depositor).



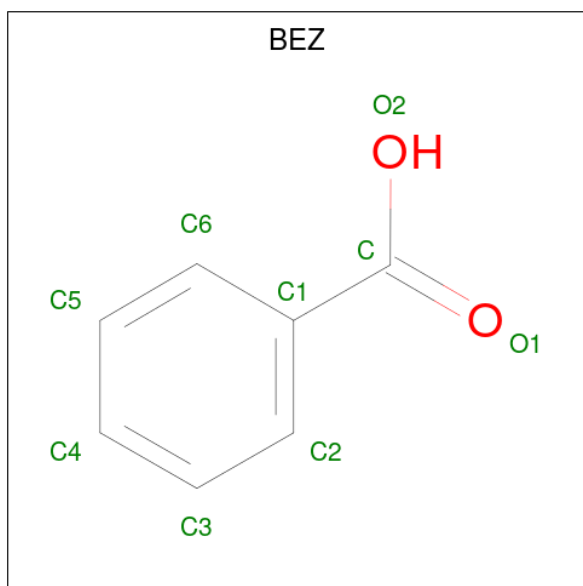
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			45	34	11		
2	B	1	Total	O	P	0	0
			45	34	11		
2	C	1	Total	O	P	0	0
			45	34	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	P	0	0
			45	34	11		

- Molecule 3 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			14	7	5	2		
3	C	1	Total	C	H	O	0	0
			14	7	5	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

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

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

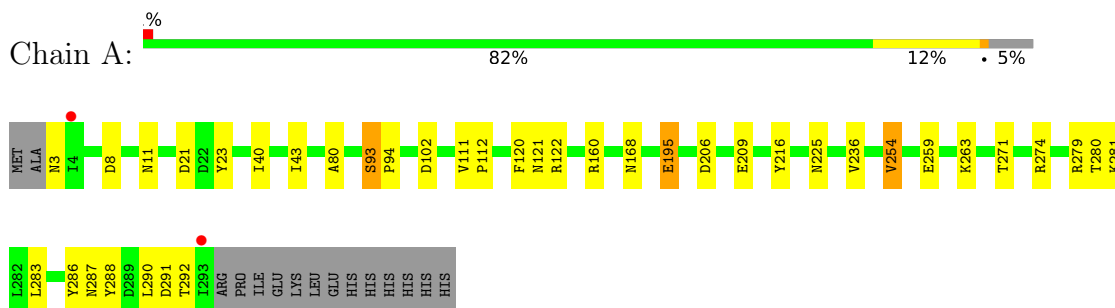
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total	O	0	0
			59	59		
6	B	48	Total	O	0	0
			48	48		
6	C	25	Total	O	0	0
			25	25		
6	D	54	Total	O	0	0
			54	54		

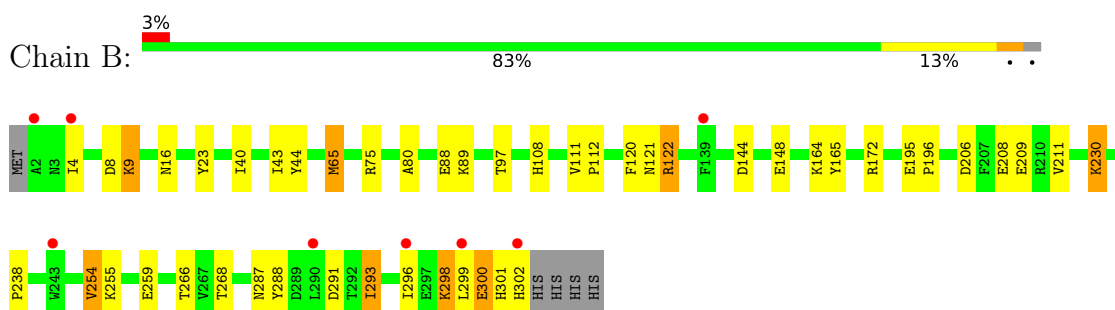
3 Residue-property plots [i](#)

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.

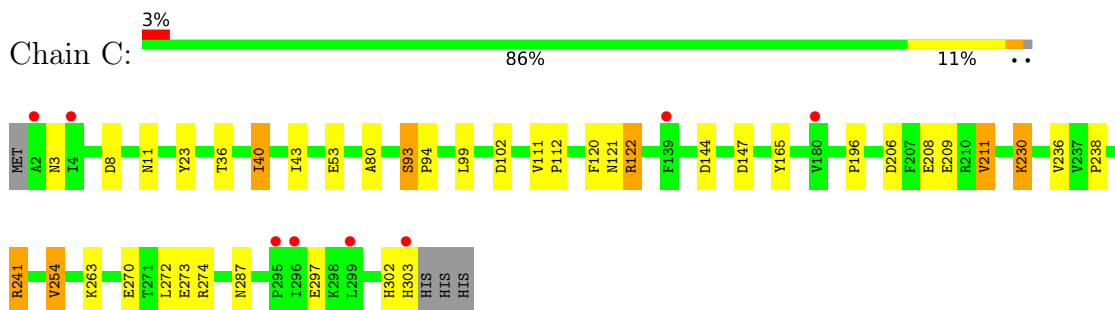
- Molecule 1: Polyphosphate--nucleotide phosphotransferase



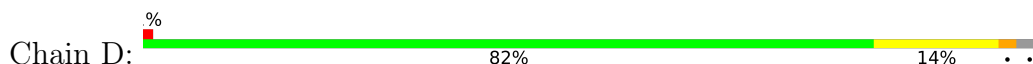
- Molecule 1: Polyphosphate--nucleotide phosphotransferase

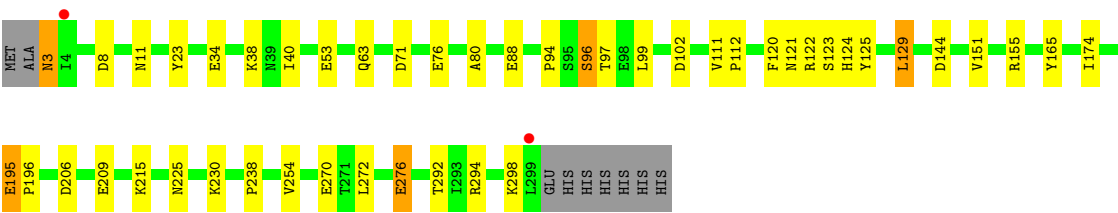


- Molecule 1: Polyphosphate--nucleotide phosphotransferase



- Molecule 1: Polyphosphate--nucleotide phosphotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.47Å 88.27Å 125.34Å 90.00° 101.15° 90.00°	Depositor
Resolution (Å)	45.11 – 2.31 45.11 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.11-2.31) 96.4 (45.11-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.176 , 0.213 0.176 , 0.213	Depositor DCC
R_{free} test set	3729 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20072	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: 6YY, BEZ, PO4, MG

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	0.94	0/2506	1.43	17/3384 (0.5%)
1	B	1.03	2/2595 (0.1%)	1.53	31/3504 (0.9%)
1	C	0.88	0/2606	1.44	19/3519 (0.5%)
1	D	1.03	1/2559 (0.0%)	1.49	25/3455 (0.7%)
All	All	0.97	3/10266 (0.0%)	1.47	92/13862 (0.7%)

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	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	302	HIS	C-O	8.49	1.40	1.23
1	B	44	TYR	C-O	-5.79	1.17	1.24
1	D	71	ASP	CG-OD1	5.39	1.35	1.25

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	34	GLU	CB-CG-CD	11.22	131.68	112.60
1	B	268	THR	CA-CB-OG1	-11.06	93.01	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	GLU	CB-CG-CD	9.99	129.59	112.60
1	C	206	ASP	CA-CB-CG	9.49	122.09	112.60
1	B	302	HIS	CA-CB-CG	9.43	123.23	113.80
1	C	3	ASN	CA-CB-CG	9.42	122.02	112.60
1	B	291	ASP	CA-CB-CG	9.34	121.94	112.60
1	B	206	ASP	CA-CB-CG	8.91	121.51	112.60
1	A	206	ASP	CA-CB-CG	8.82	121.42	112.60
1	D	206	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	287	ASN	CA-CB-CG	-8.25	104.35	112.60
1	D	298	LYS	CB-CA-C	-8.20	93.75	109.66
1	C	273	GLU	CB-CG-CD	8.04	126.26	112.60
1	B	120	PHE	CA-CB-CG	7.90	121.70	113.80
1	A	3	ASN	CB-CA-C	7.72	124.77	110.10
1	B	8	ASP	CA-CB-CG	7.69	120.29	112.60
1	A	280	THR	CA-CB-OG1	-7.64	98.14	109.60
1	C	303	HIS	CA-CB-CG	7.61	121.41	113.80
1	B	301	HIS	CA-C-O	-7.48	112.78	120.71
1	D	3	ASN	CA-CB-CG	7.46	120.06	112.60
1	C	230	LYS	CA-CB-CG	7.44	128.98	114.10
1	D	38	LYS	N-CA-CB	7.35	121.04	110.16
1	D	120	PHE	CA-CB-CG	7.28	121.08	113.80
1	D	11	ASN	CA-CB-CG	-7.16	105.44	112.60
1	D	97	THR	CA-CB-OG1	-7.09	98.96	109.60
1	B	9	LYS	CB-CG-CD	7.04	127.49	111.30
1	C	302	HIS	CA-CB-CG	7.02	120.82	113.80
1	A	120	PHE	CA-CB-CG	6.87	120.67	113.80
1	B	16	ASN	CB-CA-C	-6.84	97.97	110.63
1	D	8	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	148	GLU	CA-C-N	-6.63	111.64	122.65
1	B	148	GLU	C-N-CA	-6.63	111.64	122.65
1	D	195	GLU	CB-CA-C	-6.55	103.68	110.17
1	C	230	LYS	CB-CG-CD	6.54	126.34	111.30
1	C	8	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	144	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	53	GLU	CB-CG-CD	6.32	123.35	112.60
1	C	120	PHE	CA-CB-CG	6.26	120.06	113.80
1	A	168	ASN	CA-CB-CG	6.17	118.77	112.60
1	C	230	LYS	N-CA-CB	6.17	119.19	110.12
1	B	302	HIS	CA-C-O	6.10	131.17	120.80
1	D	215	LYS	CG-CD-CE	6.09	125.30	111.30
1	B	287	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	C	147	ASP	CA-CB-CG	6.05	118.66	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	195	GLU	CB-CA-C	-5.88	104.35	110.17
1	D	298	LYS	N-CA-CB	5.87	120.71	111.20
1	B	164	LYS	CB-CG-CD	5.81	124.66	111.30
1	D	38	LYS	CB-CA-C	-5.78	101.03	110.85
1	B	259	GLU	CB-CA-C	-5.77	101.21	110.79
1	D	144	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	11	ASN	CA-CB-CG	-5.73	106.87	112.60
1	D	238	PRO	CB-CA-C	-5.69	104.48	111.64
1	D	230	LYS	N-CA-CB	-5.67	101.55	110.06
1	D	34	GLU	CG-CD-OE2	5.67	131.44	118.40
1	B	172	ARG	CB-CA-C	-5.64	99.95	109.83
1	B	238	PRO	CB-CA-C	-5.61	104.57	111.64
1	D	53	GLU	CB-CG-CD	5.58	122.09	112.60
1	C	144	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	96	SER	CA-CB-OG	-5.50	100.10	111.10
1	A	274	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	B	88	GLU	CB-CG-CD	5.46	121.88	112.60
1	B	97	THR	CA-CB-OG1	-5.43	101.46	109.60
1	C	11	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	160	ARG	N-CA-CB	5.34	117.96	110.12
1	B	122	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	236	VAL	N-CA-CB	-5.33	104.75	111.41
1	A	225	ASN	CA-CB-CG	-5.32	107.28	112.60
1	B	300	GLU	CB-CG-CD	5.31	121.63	112.60
1	C	238	PRO	CB-CA-C	-5.30	104.96	111.64
1	C	236	VAL	N-CA-CB	-5.27	104.82	111.41
1	D	34	GLU	OE1-CD-OE2	-5.26	110.27	122.90
1	A	259	GLU	CB-CA-C	-5.25	102.07	110.79
1	B	89	LYS	CG-CD-CE	-5.24	99.24	111.30
1	D	276	GLU	CB-CG-CD	5.23	121.49	112.60
1	B	209	GLU	CG-CD-OE1	5.23	130.42	118.40
1	B	230	LYS	CB-CA-C	-5.21	102.14	110.79
1	A	291	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	122	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	D	88	GLU	CB-CG-CD	5.16	121.36	112.60
1	A	271	THR	CA-CB-OG1	-5.15	101.88	109.60
1	D	225	ASN	CA-CB-CG	-5.14	107.46	112.60
1	B	298	LYS	CA-C-O	-5.12	114.46	120.20
1	B	268	THR	OG1-CB-CG2	5.09	119.49	109.30
1	A	21	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	301	HIS	CB-CA-C	5.05	118.47	109.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	270	GLU	N-CA-CB	5.05	117.72	110.20
1	C	297	GLU	N-CA-CB	-5.02	102.74	110.12
1	C	287	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	B	255	LYS	N-CA-CB	5.01	118.04	110.28
1	B	266	THR	N-CA-C	-5.01	101.55	109.76
1	D	76	GLU	CB-CA-C	5.00	120.27	110.67

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ARG	Sidechain
1	B	300	GLU	Peptide
1	B	75	ARG	Sidechain
1	C	241	ARG	Sidechain
1	C	274	ARG	Sidechain
1	D	155	ARG	Sidechain

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	2451	2347	2400	10	0
1	B	2537	2431	2486	10	0
1	C	2547	2437	2493	11	0
1	D	2503	2408	2461	13	0
2	A	45	0	0	1	0
2	B	45	0	0	1	0
2	C	45	0	0	2	1
2	D	45	0	0	4	0
3	B	9	5	5	1	0
3	C	9	5	5	0	0
4	B	5	0	0	1	0
4	D	10	0	0	3	1
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	59	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	48	0	0	0	0
6	C	25	0	0	1	0
6	D	54	0	0	1	0
All	All	10439	9633	9850	49	2

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 2.

All (49) 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:283:LEU:O	1:A:286:TYR:O	1.99	0.80
1:B:65:MET:HA	1:B:65:MET:HE2	1.63	0.80
2:A:401:6YY:O43	2:A:401:6YY:O06	2.09	0.70
1:D:63:GLN:NE2	1:D:123:SER:HB3	2.07	0.69
1:D:40:ILE:HG23	1:D:80:ALA:HB2	1.77	0.66
2:D:401:6YY:P32	4:D:402:PO4:O3	2.54	0.66
1:A:40:ILE:HG23	1:A:80:ALA:HB2	1.78	0.65
1:B:43:ILE:HG13	1:B:254:VAL:HG23	1.80	0.63
2:B:401:6YY:O34	4:B:403:PO4:O3	2.15	0.63
1:D:63:GLN:HE21	1:D:123:SER:HB3	1.64	0.63
2:D:401:6YY:O33	4:D:402:PO4:O3	2.19	0.60
1:A:43:ILE:HG13	1:A:254:VAL:HG23	1.84	0.59
1:A:40:ILE:HG23	1:A:80:ALA:CB	2.34	0.57
1:D:40:ILE:HG23	1:D:80:ALA:CB	2.36	0.56
1:C:36:THR:O	1:C:40:ILE:HD13	2.06	0.55
1:C:102:ASP:OD2	1:D:165:TYR:OH	2.17	0.52
1:D:125:TYR:O	1:D:129:LEU:HD22	2.12	0.50
1:C:40:ILE:HG23	1:C:80:ALA:HB2	1.93	0.50
1:C:43:ILE:HG13	1:C:254:VAL:HG23	1.94	0.50
1:C:121:ASN:O	1:C:122:ARG:HB2	2.11	0.49
1:D:121:ASN:O	1:D:122:ARG:HB2	2.12	0.49
1:B:208:GLU:O	1:B:211:VAL:HG22	2.11	0.49
1:A:286:TYR:O	1:A:288:TYR:N	2.47	0.48
1:C:208:GLU:O	1:C:211:VAL:HG23	2.14	0.48
1:B:40:ILE:HG23	1:B:80:ALA:HB2	1.96	0.47
1:D:111:VAL:HG13	1:D:112:PRO:HD2	1.96	0.47
1:D:123:SER:OG	1:D:124:HIS:N	2.47	0.46
1:A:102:ASP:OD2	1:B:165:TYR:OH	2.32	0.46
2:D:401:6YY:O34	4:D:402:PO4:O1	2.34	0.45
1:B:121:ASN:O	1:B:122:ARG:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:6YY:O37	2:C:401:6YY:O22	2.34	0.45
1:B:293:ILE:HD12	1:B:293:ILE:HA	1.79	0.44
1:B:111:VAL:HG13	1:B:112:PRO:HD2	1.99	0.44
1:A:209:GLU:OE1	1:A:216:TYR:OH	2.30	0.44
1:C:165:TYR:OH	1:D:102:ASP:OD2	2.30	0.44
1:A:111:VAL:HG13	1:A:112:PRO:HD2	1.99	0.44
1:C:241:ARG:HH11	1:C:241:ARG:HG3	1.83	0.44
1:C:93:SER:HA	1:C:94:PRO:HD3	1.91	0.43
1:D:94:PRO:HB2	1:D:99:LEU:HG	2.00	0.43
1:C:94:PRO:HB2	1:C:99:LEU:HG	2.01	0.43
1:C:111:VAL:HG13	1:C:112:PRO:HD2	2.01	0.43
1:D:276:GLU:OE2	1:D:294:ARG:NH2	2.52	0.43
1:A:121:ASN:O	1:A:122:ARG:HB2	2.19	0.42
1:D:174:ILE:HA	6:D:510:HOH:O	2.18	0.42
1:B:108:HIS:ND1	3:B:402:BEZ:H4	2.35	0.41
1:B:288:TYR:O	1:B:298:LYS:HE3	2.20	0.41
2:D:401:6YY:O36	2:D:401:6YY:O27	2.38	0.41
1:A:93:SER:HA	1:A:94:PRO:HD3	1.88	0.41
2:C:401:6YY:O42	6:C:501:HOH:O	2.22	0.40

All (2) 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)
2:C:401:6YY:O03	2:C:401:6YY:O03[2_656]	2.02	0.18
4:D:403:PO4:O2	4:D:403:PO4:O2[2_555]	2.18	0.02

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	289/306 (94%)	279 (96%)	10 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	299/306 (98%)	285 (95%)	14 (5%)	0	100	100
1	C	300/306 (98%)	290 (97%)	10 (3%)	0	100	100
1	D	295/306 (96%)	286 (97%)	9 (3%)	0	100	100
All	All	1183/1224 (97%)	1140 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	268/282 (95%)	260 (97%)	8 (3%)	36	52
1	B	277/282 (98%)	266 (96%)	11 (4%)	28	41
1	C	278/282 (99%)	267 (96%)	11 (4%)	28	41
1	D	274/282 (97%)	263 (96%)	11 (4%)	28	41
All	All	1097/1128 (97%)	1056 (96%)	41 (4%)	30	44

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	93	SER
1	A	195	GLU
1	A	254	VAL
1	A	263	LYS
1	A	281	LYS
1	A	290	LEU
1	A	292	THR
1	B	4	ILE
1	B	9	LYS
1	B	23	TYR
1	B	65	MET
1	B	195	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	196	PRO
1	B	230	LYS
1	B	254	VAL
1	B	293	ILE
1	B	296	ILE
1	B	299	LEU
1	C	23	TYR
1	C	40	ILE
1	C	93	SER
1	C	196	PRO
1	C	209	GLU
1	C	211	VAL
1	C	230	LYS
1	C	254	VAL
1	C	263	LYS
1	C	270	GLU
1	C	272	LEU
1	D	3	ASN
1	D	23	TYR
1	D	96	SER
1	D	129	LEU
1	D	151	VAL
1	D	195	GLU
1	D	196	PRO
1	D	209	GLU
1	D	254	VAL
1	D	272	LEU
1	D	292	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	18	HIS
1	A	63	GLN
1	A	161	ASN
1	A	168	ASN
1	A	217	GLN
1	B	87	HIS
1	B	109	ASN
1	B	169	ASN
1	B	217	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	HIS
1	C	16	ASN
1	C	63	GLN
1	C	109	ASN
1	C	301	HIS
1	D	3	ASN
1	D	12	ASN
1	D	18	HIS
1	D	63	GLN
1	D	87	HIS
1	D	217	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BEZ	B	402	-	9,9,9	3.35	1 (11%)	11,11,11	2.77	5 (45%)
2	6YY	A	401	-	42,44,44	2.81	13 (30%)	57,76,76	3.37	27 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	B	403	-	4,4,4	2.53	1 (25%)	6,6,6	0.71	0
4	PO4	D	402	-	4,4,4	3.98	3 (75%)	6,6,6	0.56	0
2	6YY	D	401	-	42,44,44	2.34	11 (26%)	57,76,76	3.07	26 (45%)
4	PO4	D	403	-	4,4,4	2.90	2 (50%)	6,6,6	1.48	1 (16%)
2	6YY	B	401	-	42,44,44	2.30	10 (23%)	57,76,76	2.61	23 (40%)
2	6YY	C	401	-	42,44,44	2.13	9 (21%)	57,76,76	2.44	23 (40%)
3	BEZ	C	402	-	9,9,9	2.17	2 (22%)	11,11,11	1.69	4 (36%)

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	BEZ	B	402	-	-	0/4/4/4	0/1/1/1
2	6YY	A	401	-	-	10/60/60/60	-
2	6YY	D	401	-	-	6/60/60/60	-
2	6YY	B	401	-	-	11/60/60/60	-
2	6YY	C	401	-	-	14/60/60/60	-
3	BEZ	C	402	-	-	0/4/4/4	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	6YY	P05-O04	11.91	1.72	1.59
3	B	402	BEZ	C1-C	-9.62	1.29	1.49
2	D	401	6YY	P29-O31	7.04	1.67	1.59
2	B	401	6YY	P26-O28	7.02	1.67	1.59
2	D	401	6YY	P32-O33	6.59	1.79	1.54
2	A	401	6YY	P02-O03	6.55	1.70	1.50
4	D	402	PO4	P-O1	6.20	1.65	1.50
2	D	401	6YY	P23-O25	5.77	1.65	1.59
2	C	401	6YY	P05-O07	5.70	1.65	1.59
2	C	401	6YY	P08-O07	5.45	1.65	1.59
2	B	401	6YY	P23-O25	5.44	1.65	1.59
3	C	402	BEZ	C1-C	-5.43	1.37	1.49
2	A	401	6YY	P02-O01	5.35	1.74	1.54
2	B	401	6YY	P29-O28	4.96	1.64	1.59
4	D	403	PO4	P-O3	4.47	1.67	1.54
2	C	401	6YY	P23-O25	4.38	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	6YY	P14-O13	4.32	1.64	1.59
2	A	401	6YY	P05-O07	4.32	1.64	1.59
2	B	401	6YY	P26-O25	4.10	1.63	1.59
4	B	403	PO4	P-O1	4.06	1.60	1.50
2	A	401	6YY	P08-O07	3.75	1.63	1.59
2	A	401	6YY	P29-O28	-3.73	1.55	1.59
2	D	401	6YY	P32-O34	3.65	1.61	1.50
2	C	401	6YY	P26-O28	-3.64	1.55	1.59
2	B	401	6YY	P29-O31	3.54	1.63	1.59
4	D	402	PO4	P-O3	3.54	1.64	1.54
2	D	401	6YY	P26-O25	3.35	1.63	1.59
4	D	402	PO4	P-O2	3.33	1.64	1.54
2	C	401	6YY	P08-O10	3.29	1.63	1.59
4	D	403	PO4	P-O1	3.22	1.58	1.50
2	A	401	6YY	P11-O10	3.16	1.62	1.59
2	C	401	6YY	P20-O22	3.07	1.62	1.59
2	D	401	6YY	P29-O28	3.06	1.62	1.59
2	B	401	6YY	P08-O07	-3.05	1.56	1.59
2	D	401	6YY	P05-O07	-2.84	1.56	1.59
2	B	401	6YY	P23-O22	2.81	1.62	1.59
2	B	401	6YY	P20-O22	2.74	1.62	1.59
2	D	401	6YY	P11-O10	2.71	1.62	1.59
3	C	402	BEZ	C2-C1	-2.57	1.35	1.39
2	C	401	6YY	P05-O04	2.42	1.62	1.59
2	D	401	6YY	P02-O01	-2.41	1.45	1.54
2	B	401	6YY	P02-O01	-2.38	1.46	1.54
2	C	401	6YY	P11-O13	2.38	1.62	1.59
2	D	401	6YY	P05-O44	-2.20	1.45	1.55
2	D	401	6YY	P14-O41	-2.19	1.45	1.55
2	A	401	6YY	P17-O19	2.18	1.61	1.59
2	A	401	6YY	P08-O10	2.16	1.61	1.59
2	A	401	6YY	P20-O19	2.14	1.61	1.59
2	A	401	6YY	P14-O16	2.07	1.61	1.59
2	A	401	6YY	P26-O28	-2.07	1.57	1.59
2	B	401	6YY	P32-O34	2.06	1.56	1.50
2	A	401	6YY	P23-O25	-2.05	1.57	1.59

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	6YY	O45-P02-O03	-11.65	65.42	110.83
2	A	401	6YY	O45-P02-O01	9.37	142.92	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	6YY	O12-P11-O13	-8.58	84.09	107.27
2	D	401	6YY	O37-P26-O25	8.14	129.26	107.27
2	D	401	6YY	O35-P32-O34	-7.66	81.00	110.83
2	B	401	6YY	O12-P11-O10	7.52	127.59	107.27
2	A	401	6YY	O16-P14-O15	-7.25	88.90	110.70
2	B	401	6YY	O37-P26-O25	-7.04	88.24	107.27
2	A	401	6YY	O07-P05-O06	-6.57	90.94	110.70
2	A	401	6YY	O01-P02-O04	6.31	125.80	104.64
2	D	401	6YY	O37-P26-O28	-6.31	90.22	107.27
2	A	401	6YY	O45-P02-O04	-6.07	84.27	104.64
2	C	401	6YY	O16-P14-O15	-6.06	92.47	110.70
2	D	401	6YY	O31-P29-O36	6.02	128.81	110.70
2	D	401	6YY	O25-P26-O27	-5.99	92.70	110.70
2	D	401	6YY	O35-P32-O33	5.98	130.23	107.80
2	D	401	6YY	O33-P32-O31	5.90	124.44	104.64
2	B	401	6YY	O13-P11-O42	-5.46	94.28	110.70
2	A	401	6YY	O04-P02-O03	5.26	138.73	111.04
2	C	401	6YY	O37-P26-O25	-5.20	93.21	107.27
2	D	401	6YY	O35-P32-O31	-5.11	87.49	104.64
2	D	401	6YY	O41-P14-O16	4.83	120.33	107.27
3	B	402	BEZ	C6-C1-C2	4.80	124.67	118.57
2	C	401	6YY	O18-P17-O16	-4.78	94.35	107.27
2	A	401	6YY	O44-P05-O04	4.69	119.95	107.27
2	C	401	6YY	O12-P11-O13	-4.52	95.06	107.27
3	B	402	BEZ	O2-C-O1	4.49	133.01	123.35
2	A	401	6YY	O01-P02-O03	-4.33	93.98	110.83
2	C	401	6YY	O30-P29-O31	4.17	118.55	107.27
2	B	401	6YY	O25-P26-O27	4.14	123.15	110.70
2	C	401	6YY	O22-P23-O24	-4.05	98.51	110.70
2	A	401	6YY	O04-P05-O06	4.04	122.86	110.70
2	A	401	6YY	O35-P32-O33	4.03	122.91	107.80
2	A	401	6YY	O12-P11-O10	3.96	117.97	107.27
2	C	401	6YY	O41-P14-O16	-3.93	96.64	107.27
2	B	401	6YY	O30-P29-O31	-3.86	96.84	107.27
2	C	401	6YY	O21-P20-O22	-3.75	97.14	107.27
2	C	401	6YY	O18-P17-O19	-3.73	97.20	107.27
2	D	401	6YY	O33-P32-O34	3.71	125.29	110.83
2	C	401	6YY	O28-P29-O36	3.71	121.85	110.70
3	B	402	BEZ	O1-C-C1	-3.63	111.93	121.46
3	B	402	BEZ	C5-C6-C1	-3.58	116.85	120.36
2	A	401	6YY	O38-P23-O25	-3.55	97.67	107.27
2	D	401	6YY	O28-P29-O36	-3.54	100.05	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	6YY	O38-P23-O22	3.54	116.85	107.27
3	B	402	BEZ	C3-C2-C1	-3.31	117.11	120.36
2	D	401	6YY	O37-P26-O27	3.30	127.78	112.44
2	D	401	6YY	O10-P08-O43	-3.27	100.88	110.70
2	A	401	6YY	O33-P32-O34	-3.25	98.18	110.83
2	D	401	6YY	O21-P20-O19	-3.19	98.65	107.27
2	C	401	6YY	O13-P14-O15	3.16	120.20	110.70
2	D	401	6YY	O19-P17-O40	-3.10	101.38	110.70
2	D	401	6YY	O22-P23-O24	-3.00	101.68	110.70
2	D	401	6YY	O19-P20-O39	-2.95	101.83	110.70
2	D	401	6YY	O31-P32-O34	-2.95	95.54	111.04
2	C	401	6YY	O01-P02-O04	2.92	114.44	104.64
3	C	402	BEZ	C6-C1-C2	2.91	122.27	118.57
2	B	401	6YY	O01-P02-O03	2.91	122.15	110.83
4	D	403	PO4	O3-P-O2	2.89	116.92	107.91
2	B	401	6YY	O41-P14-O16	2.88	115.07	107.27
2	C	401	6YY	O18-P17-O40	2.86	125.77	112.44
2	B	401	6YY	O35-P32-O31	2.84	114.16	104.64
2	C	401	6YY	O07-P08-O43	-2.83	102.18	110.70
2	D	401	6YY	O44-P05-O04	2.76	114.74	107.27
3	C	402	BEZ	O1-C-C1	-2.75	114.25	121.46
2	B	401	6YY	O16-P17-O40	-2.75	102.44	110.70
2	A	401	6YY	O09-P08-O07	-2.74	99.86	107.27
2	D	401	6YY	O22-P20-O39	2.72	118.88	110.70
2	B	401	6YY	O25-P23-O24	2.70	118.84	110.70
2	C	401	6YY	O19-P17-O40	2.70	118.82	110.70
2	B	401	6YY	O44-P05-O04	-2.67	100.06	107.27
2	D	401	6YY	O09-P08-O07	2.65	114.44	107.27
2	A	401	6YY	O38-P23-O24	2.65	124.76	112.44
2	B	401	6YY	O12-P11-O42	2.62	124.64	112.44
2	C	401	6YY	O09-P08-O07	2.62	114.35	107.27
2	A	401	6YY	O21-P20-O19	2.61	114.33	107.27
2	A	401	6YY	O13-P11-O42	2.59	118.51	110.70
2	B	401	6YY	O16-P14-O15	-2.57	102.96	110.70
2	A	401	6YY	O41-P14-O15	2.57	124.41	112.44
2	C	401	6YY	O21-P20-O19	2.57	114.22	107.27
2	D	401	6YY	O38-P23-O22	-2.56	100.34	107.27
2	D	401	6YY	O12-P11-O10	2.54	114.14	107.27
2	A	401	6YY	O37-P26-O28	2.54	114.14	107.27
3	C	402	BEZ	C5-C6-C1	-2.50	117.91	120.36
2	B	401	6YY	O37-P26-O28	2.47	113.94	107.27
2	A	401	6YY	O12-P11-O13	-2.45	100.64	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	6YY	O31-P32-O34	-2.38	98.50	111.04
2	B	401	6YY	O18-P17-O40	2.38	123.50	112.44
2	A	401	6YY	O41-P14-O13	2.35	113.63	107.27
2	D	401	6YY	O21-P20-O39	2.34	123.34	112.44
2	B	401	6YY	O44-P05-O06	2.34	123.32	112.44
2	A	401	6YY	O30-P29-O36	2.34	123.32	112.44
2	D	401	6YY	O30-P29-O31	-2.33	100.97	107.27
2	B	401	6YY	O28-P26-O27	-2.21	104.06	110.70
2	B	401	6YY	O44-P05-O07	2.20	113.23	107.27
2	C	401	6YY	O31-P29-O36	-2.19	104.12	110.70
2	B	401	6YY	O07-P08-O43	2.18	117.25	110.70
2	C	401	6YY	O30-P29-O28	-2.16	101.44	107.27
2	A	401	6YY	O25-P23-O24	2.15	117.18	110.70
2	C	401	6YY	O41-P14-O15	2.15	122.46	112.44
2	B	401	6YY	O09-P08-O10	-2.13	101.52	107.27
2	D	401	6YY	O12-P11-O13	-2.11	101.56	107.27
3	C	402	BEZ	O2-C-O1	2.11	127.89	123.35
2	C	401	6YY	O45-P02-O04	-2.10	97.58	104.64
2	B	401	6YY	O21-P20-O39	2.06	122.02	112.44
2	A	401	6YY	O37-P26-O27	2.03	121.88	112.44
2	A	401	6YY	O35-P32-O31	2.02	111.41	104.64
2	A	401	6YY	O10-P08-O43	-2.01	104.65	110.70
2	C	401	6YY	O45-P02-O03	2.00	118.64	110.83

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	6YY	P05-O04-P02-O45
2	D	401	6YY	P05-O04-P02-O01
2	B	401	6YY	P20-O19-P17-O40
2	C	401	6YY	P02-O04-P05-O06
2	C	401	6YY	P11-O10-P08-O07
2	C	401	6YY	P29-O31-P32-O34
2	B	401	6YY	P29-O31-P32-O33
2	A	401	6YY	P26-O28-P29-O30
2	B	401	6YY	P20-O19-P17-O18
2	B	401	6YY	P20-O22-P23-O24
2	B	401	6YY	P23-O25-P26-O37
2	C	401	6YY	P20-O19-P17-O18
2	A	401	6YY	P02-O04-P05-O06
2	A	401	6YY	P14-O13-P11-O42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	401	6YY	P29-O31-P32-O34
2	B	401	6YY	P05-O04-P02-O03
2	C	401	6YY	P05-O04-P02-O01
2	C	401	6YY	P29-O31-P32-O33
2	C	401	6YY	P29-O31-P32-O35
2	A	401	6YY	P11-O10-P08-O09
2	B	401	6YY	P20-O22-P23-O38
2	B	401	6YY	P26-O25-P23-O38
2	B	401	6YY	P26-O28-P29-O30
2	C	401	6YY	P02-O04-P05-O44
2	C	401	6YY	P17-O16-P14-O41
2	C	401	6YY	P20-O19-P17-O40
2	C	401	6YY	P23-O22-P20-O21
2	D	401	6YY	P08-O07-P05-O06
2	D	401	6YY	P08-O07-P05-O44
2	D	401	6YY	P26-O25-P23-O24
2	D	401	6YY	P26-O25-P23-O38
2	D	401	6YY	P26-O28-P29-O30
2	A	401	6YY	P08-O07-P05-O44
2	A	401	6YY	P11-O10-P08-O43
2	A	401	6YY	P14-O13-P11-O12
2	A	401	6YY	P14-O16-P17-O18
2	A	401	6YY	P26-O28-P29-O36
2	B	401	6YY	P08-O07-P05-O44
2	C	401	6YY	P05-O07-P08-O09
2	C	401	6YY	P11-O10-P08-O09
2	C	401	6YY	P11-O10-P08-O43

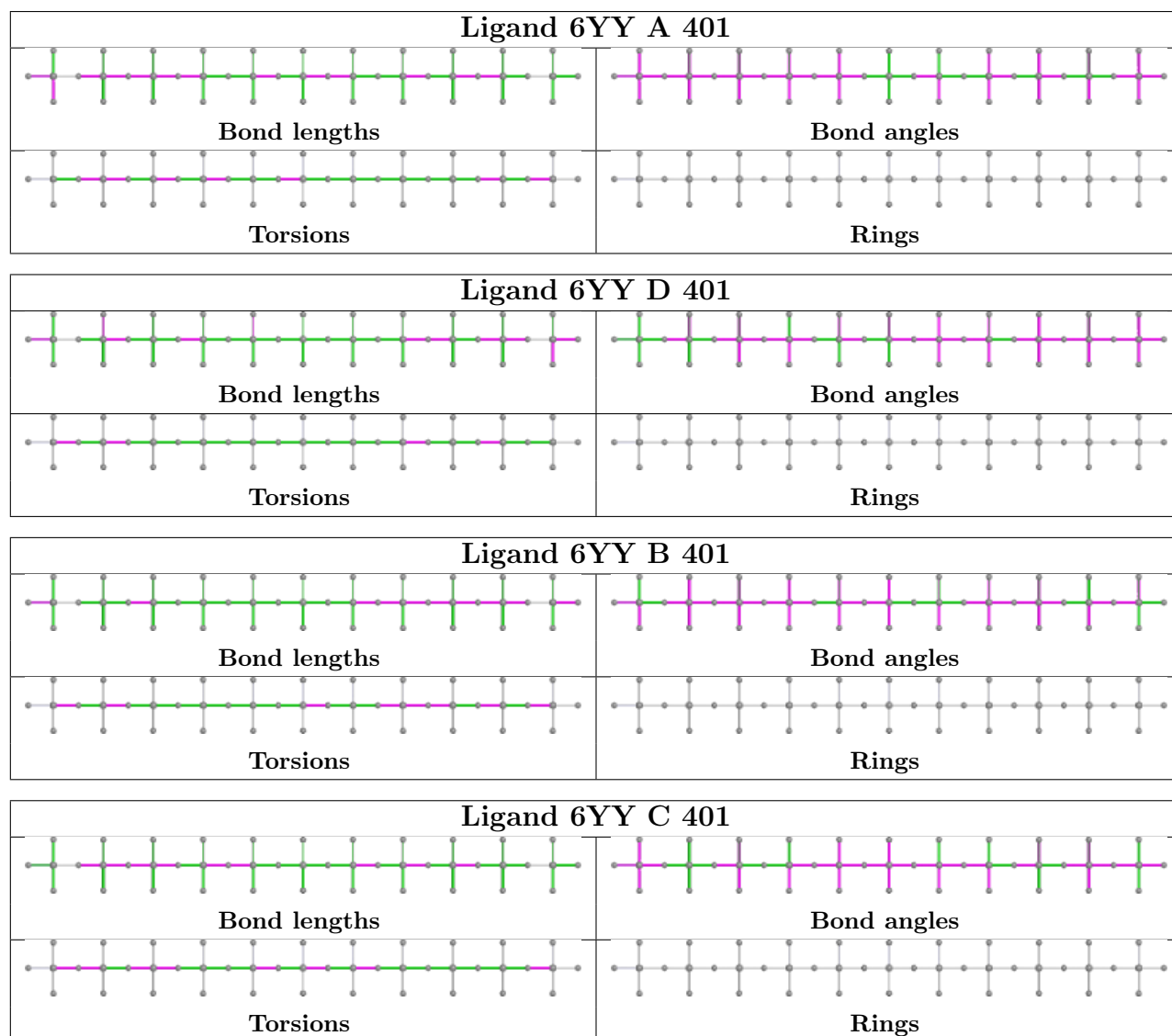
There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	BEZ	1	0
2	A	401	6YY	1	0
4	B	403	PO4	1	0
4	D	402	PO4	3	0
2	D	401	6YY	4	0
4	D	403	PO4	0	1
2	B	401	6YY	1	0
2	C	401	6YY	2	1

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	291/306 (95%)	-0.43	2 (0%) 84 85	44, 61, 116, 146	0
1	B	301/306 (98%)	-0.32	8 (2%) 56 59	43, 63, 92, 145	0
1	C	302/306 (98%)	-0.15	8 (2%) 57 60	50, 75, 107, 148	0
1	D	297/306 (97%)	-0.41	2 (0%) 84 85	42, 58, 91, 133	0
All	All	1191/1224 (97%)	-0.33	20 (1%) 69 71	42, 64, 106, 148	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	299	LEU	6.3
1	C	303	HIS	4.8
1	D	4	ILE	4.7
1	A	293	ILE	4.6
1	C	296	ILE	3.6
1	C	2	ALA	3.1
1	B	243	TRP	2.8
1	B	2	ALA	2.8
1	B	302	HIS	2.6
1	C	139	PHE	2.6
1	B	4	ILE	2.5
1	C	299	LEU	2.4
1	B	290	LEU	2.4
1	B	299	LEU	2.3
1	C	4	ILE	2.3
1	B	296	ILE	2.3
1	C	295	PRO	2.2
1	C	180	VAL	2.1
1	A	4	ILE	2.1
1	B	139	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

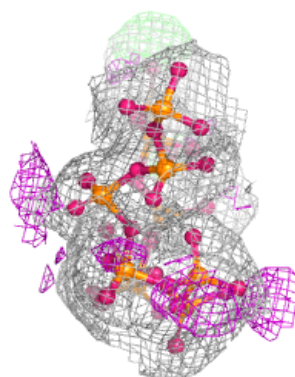
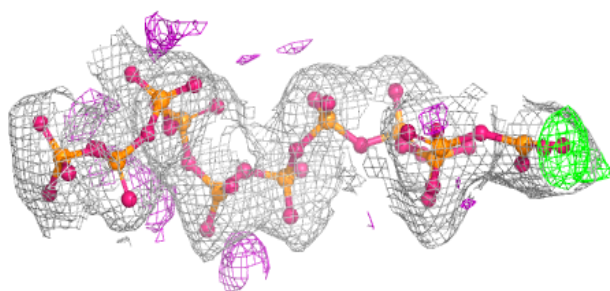
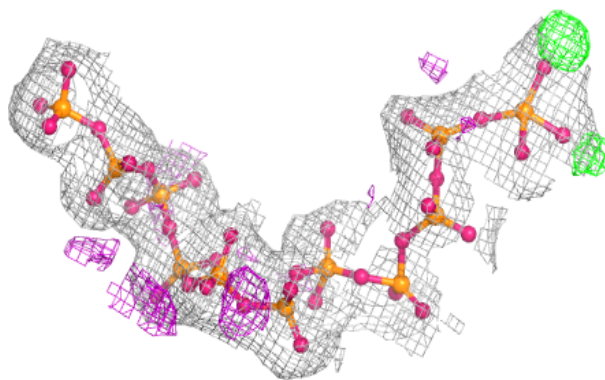
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	B	403	5/5	0.58	0.08	91,105,119,143	0
4	PO4	D	402	5/5	0.86	0.06	78,81,104,123	0
5	MG	D	404	1/1	0.86	0.10	62,62,62,62	0
4	PO4	D	403	5/5	0.89	0.09	70,84,107,121	0
5	MG	C	403	1/1	0.92	0.06	67,67,67,67	0
2	6YY	A	401	45/45	0.95	0.06	47,62,100,132	0
2	6YY	C	401	45/45	0.96	0.06	64,80,145,169	0
2	6YY	D	401	45/45	0.97	0.05	37,53,102,112	0
3	BEZ	B	402	9/9	0.97	0.08	42,53,60,65	0
3	BEZ	C	402	9/9	0.97	0.10	49,63,67,67	0
2	6YY	B	401	45/45	0.97	0.05	48,58,124,127	0

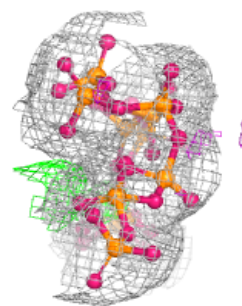
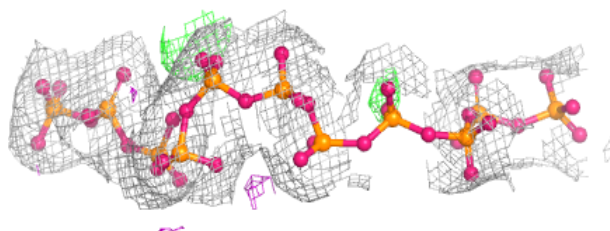
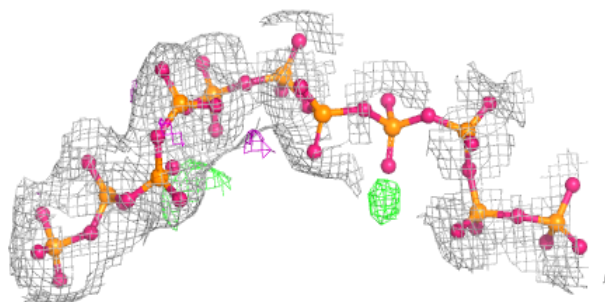
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6YY A 401:

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

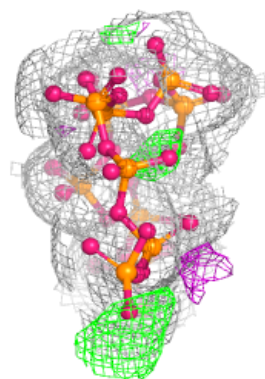
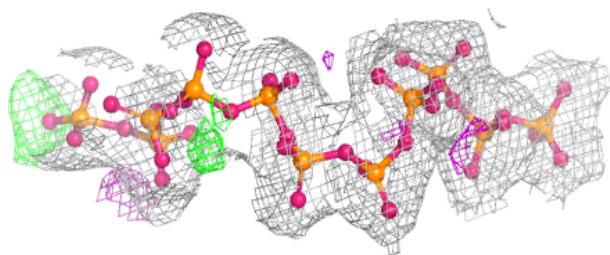
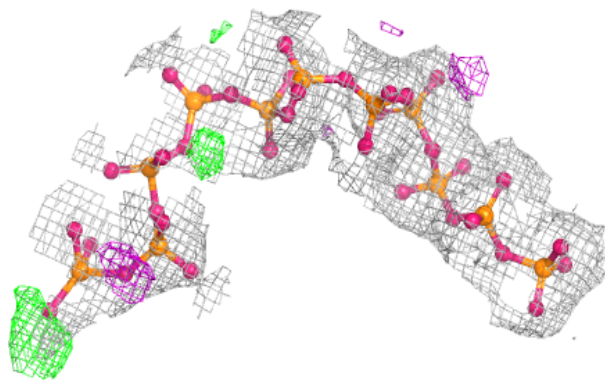
**Electron density around 6YY C 401:**

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

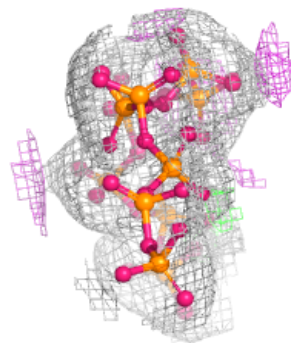
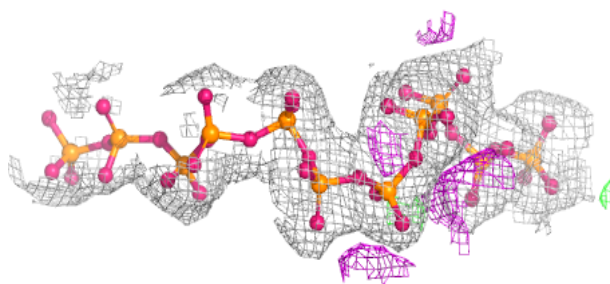
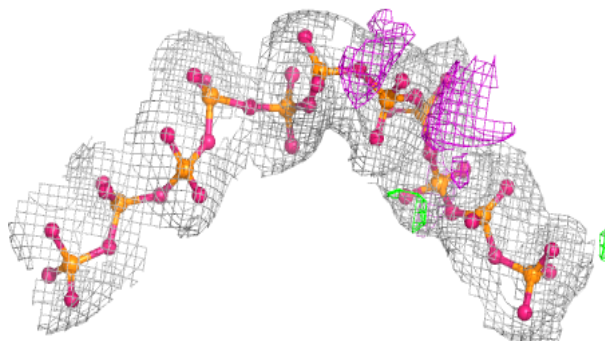


Electron density around 6YY D 401:

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

**Electron density around 6YY B 401:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.