



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:06 PM GMT

PDB ID : 1E33
Title : CRYSTAL STRUCTURE OF AN ARYLSULFATASE A MUTANT P426L
Authors : Von Buelow, R.; Schmidt, B.; Dierks, T.; Von Figura, K.; Uson, I.
Deposited on : 2000-06-06
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

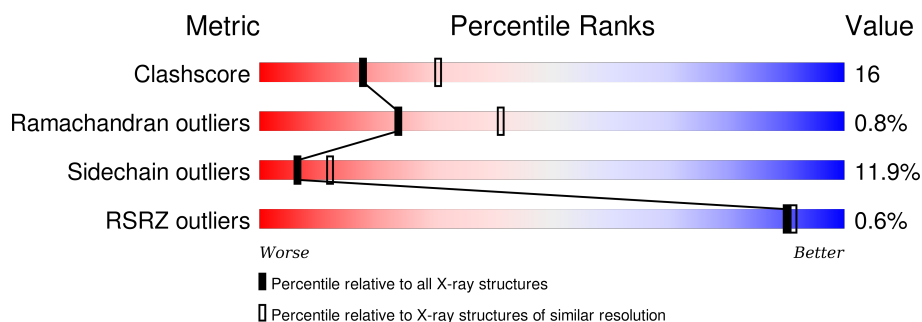
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	P	489	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3754 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 ARYLSULFATASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	481	Total	C	N	O	S	0	0	0
			3555	2269	602	661	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	215	GLU	GLN	CONFLICT	UNP P15289
P	426	LEU	PRO	ENGINEERED MUTATION	UNP P15289

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Mg	0	0
			1	1		

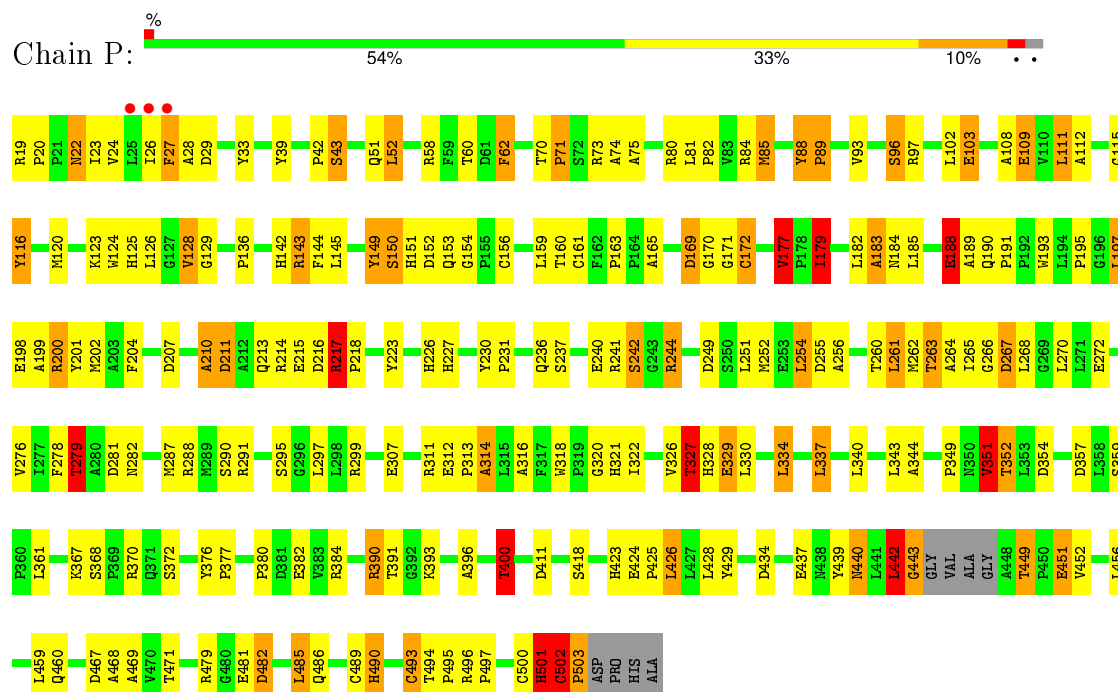
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	170	Total	O	0	0
			170	170		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ARYLSULFATASE A



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.40 Å 131.40 Å 192.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.50) 99.2 (29.48-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.250 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.9	EDS
Estimated twinning fraction	0.017 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.005 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 29156 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3754	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	P	1.02	2/3653 (0.1%)	2.38	172/4991 (3.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	295	SER	CB-OG	6.61	1.50	1.42
1	P	503	PRO	N-CD	6.50	1.56	1.47

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	244	ARG	NE-CZ-NH1	27.60	134.10	120.30
1	P	291	ARG	NE-CZ-NH2	-27.46	106.57	120.30
1	P	288	ARG	NE-CZ-NH2	19.32	129.96	120.30
1	P	109	GLU	OE1-CD-OE2	-17.08	102.80	123.30
1	P	143	ARG	NE-CZ-NH2	-16.83	111.89	120.30
1	P	496	ARG	NE-CZ-NH1	16.37	128.49	120.30
1	P	73	ARG	NE-CZ-NH1	-15.63	112.48	120.30
1	P	73	ARG	CD-NE-CZ	15.18	144.84	123.60
1	P	390	ARG	NE-CZ-NH1	14.69	127.64	120.30
1	P	33	TYR	CB-CG-CD2	-14.10	112.54	121.00
1	P	244	ARG	NH1-CZ-NH2	-13.49	104.56	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	390	ARG	NE-CZ-NH2	-13.47	113.56	120.30
1	P	33	TYR	CB-CG-CD1	13.24	128.95	121.00
1	P	97	ARG	NE-CZ-NH2	13.22	126.91	120.30
1	P	439	TYR	CB-CG-CD2	12.90	128.74	121.00
1	P	200	ARG	NE-CZ-NH1	12.31	126.46	120.30
1	P	479	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	P	29	ASP	CB-CG-OD2	12.14	129.23	118.30
1	P	200	ARG	NE-CZ-NH2	-12.05	114.27	120.30
1	P	496	ARG	CD-NE-CZ	11.46	139.65	123.60
1	P	299	ARG	NE-CZ-NH1	-11.17	114.72	120.30
1	P	80	ARG	NE-CZ-NH2	11.15	125.88	120.30
1	P	143	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	P	291	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	P	217	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	P	179	ILE	CA-CB-CG2	10.34	131.57	110.90
1	P	230	TYR	CB-CG-CD1	-10.16	114.90	121.00
1	P	267	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	P	479	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	P	143	ARG	CD-NE-CZ	9.53	136.94	123.60
1	P	230	TYR	CB-CG-CD2	9.46	126.67	121.00
1	P	80	ARG	NE-CZ-NH1	-9.35	115.63	120.30
1	P	496	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	P	207	ASP	CB-CG-OD2	-9.32	109.91	118.30
1	P	439	TYR	CB-CG-CD1	-9.23	115.46	121.00
1	P	329	GLU	OE1-CD-OE2	9.20	134.34	123.30
1	P	311	ARG	CD-NE-CZ	9.17	136.44	123.60
1	P	97	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	P	370	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	P	489	CYS	C-N-CA	9.08	144.40	121.70
1	P	411	ASP	CB-CG-OD2	-9.07	110.13	118.30
1	P	426	LEU	CA-CB-CG	9.02	136.05	115.30
1	P	391	THR	OG1-CB-CG2	-8.84	89.68	110.00
1	P	337	LEU	CA-CB-CG	8.69	135.28	115.30
1	P	314	ALA	CB-CA-C	8.55	122.93	110.10
1	P	210	ALA	CB-CA-C	8.32	122.58	110.10
1	P	84	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	P	489	CYS	CA-CB-SG	-8.23	99.18	114.00
1	P	299	ARG	NH1-CZ-NH2	8.03	128.23	119.40
1	P	242	SER	C-N-CA	-7.94	105.62	122.30
1	P	108	ALA	CB-CA-C	7.91	121.97	110.10
1	P	291	ARG	NH1-CZ-NH2	7.75	127.93	119.40
1	P	311	ARG	NE-CZ-NH1	-7.61	116.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	58	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	P	177	VAL	N-CA-CB	-7.50	95.01	111.50
1	P	242	SER	CA-C-N	7.45	131.10	116.20
1	P	288	ARG	NH1-CZ-NH2	-7.44	111.22	119.40
1	P	429	TYR	O-C-N	7.43	134.59	122.70
1	P	255	ASP	CB-CG-OD1	7.41	124.97	118.30
1	P	149	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	P	281	ASP	CB-CG-OD1	7.40	124.96	118.30
1	P	327	THR	CB-CA-C	-7.35	91.77	111.60
1	P	434	ASP	CB-CG-OD1	7.30	124.87	118.30
1	P	109	GLU	CG-CD-OE1	7.28	132.86	118.30
1	P	311	ARG	CG-CD-NE	7.28	127.08	111.80
1	P	326	VAL	CG1-CB-CG2	-7.25	99.30	110.90
1	P	481	GLU	OE1-CD-OE2	7.19	131.93	123.30
1	P	384	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	P	287	MET	N-CA-CB	-7.14	97.74	110.60
1	P	494	THR	CA-C-O	-7.14	105.11	120.10
1	P	494	THR	O-C-N	7.14	134.66	121.10
1	P	354	ASP	CB-CG-OD1	7.13	124.72	118.30
1	P	249	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	P	27	PHE	CB-CG-CD1	6.96	125.67	120.80
1	P	39	TYR	N-CA-CB	6.89	123.00	110.60
1	P	376	TYR	CB-CG-CD1	6.77	125.06	121.00
1	P	391	THR	CA-CB-OG1	-6.71	94.91	109.00
1	P	443	GLY	CA-C-O	6.70	132.66	120.60
1	P	299	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	P	352	THR	C-N-CA	6.62	138.25	121.70
1	P	73	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	P	279	THR	CB-CA-C	-6.55	93.90	111.60
1	P	116	TYR	CB-CG-CD1	6.55	124.93	121.00
1	P	425	PRO	N-CA-CB	6.55	111.16	103.30
1	P	411	ASP	CB-CG-OD1	6.53	124.17	118.30
1	P	279	THR	N-CA-CB	6.50	122.65	110.30
1	P	467	ASP	CB-CG-OD1	6.48	124.13	118.30
1	P	281	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	P	497	PRO	CA-N-CD	-6.38	102.56	111.50
1	P	344	ALA	O-C-N	-6.36	112.39	123.20
1	P	43	SER	N-CA-CB	6.36	120.04	110.50
1	P	494	THR	N-CA-CB	6.35	122.36	110.30
1	P	307	GLU	OE1-CD-OE2	6.27	130.83	123.30
1	P	376	TYR	CG-CD1-CE1	6.23	126.28	121.30
1	P	171	GLY	N-CA-C	6.22	128.65	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	193	TRP	CB-CG-CD1	6.21	135.07	127.00
1	P	376	TYR	CA-CB-CG	6.20	125.17	113.40
1	P	424	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	P	177	VAL	CA-CB-CG1	6.14	120.11	110.90
1	P	384	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	P	179	ILE	CA-CB-CG1	-6.03	99.55	111.00
1	P	170	GLY	C-N-CA	-6.01	109.68	122.30
1	P	490	HIS	N-CA-CB	5.98	121.37	110.60
1	P	62	PHE	O-C-N	-5.97	113.15	122.70
1	P	116	TYR	CA-CB-CG	5.97	124.74	113.40
1	P	52	LEU	N-CA-CB	-5.94	98.53	110.40
1	P	312	GLU	CG-CD-OE1	5.84	129.98	118.30
1	P	169	ASP	CB-CG-OD2	5.82	123.54	118.30
1	P	426	LEU	N-CA-CB	-5.78	98.83	110.40
1	P	52	LEU	CB-CA-C	5.76	121.14	110.20
1	P	197	LEU	O-C-N	-5.75	113.49	122.70
1	P	211	ASP	O-C-N	-5.75	113.50	122.70
1	P	200	ARG	CD-NE-CZ	5.73	131.62	123.60
1	P	244	ARG	CD-NE-CZ	-5.72	115.59	123.60
1	P	496	ARG	CA-C-O	-5.72	108.09	120.10
1	P	33	TYR	CA-C-N	5.66	127.52	116.20
1	P	193	TRP	CB-CG-CD2	-5.66	119.24	126.60
1	P	437	GLU	CA-CB-CG	5.66	125.84	113.40
1	P	84	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	P	251	LEU	CA-CB-CG	5.60	128.18	115.30
1	P	400	THR	N-CA-CB	-5.58	99.69	110.30
1	P	242	SER	CA-C-O	-5.58	108.39	120.10
1	P	215	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	P	249	ASP	CB-CG-OD1	5.54	123.29	118.30
1	P	482	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	P	351	VAL	O-C-N	5.49	131.48	122.70
1	P	382	GLU	OE1-CD-OE2	5.49	129.88	123.30
1	P	62	PHE	CB-CG-CD2	5.48	124.63	120.80
1	P	456	LEU	CA-CB-CG	5.47	127.88	115.30
1	P	442	LEU	CA-C-N	5.44	127.07	116.20
1	P	103	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	P	170	GLY	N-CA-C	5.41	126.63	113.10
1	P	418	SER	N-CA-CB	5.39	118.59	110.50
1	P	154	GLY	N-CA-C	-5.38	99.64	113.10
1	P	169	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	P	351	VAL	CB-CA-C	-5.38	101.19	111.40
1	P	469	ALA	CB-CA-C	-5.38	102.04	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	120	MET	CG-SD-CE	-5.36	91.62	100.20
1	P	210	ALA	O-C-N	-5.34	114.15	122.70
1	P	320	GLY	CA-C-O	-5.34	110.99	120.60
1	P	263	THR	CA-CB-CG2	-5.34	104.93	112.40
1	P	217	ARG	NH1-CZ-NH2	-5.33	113.53	119.40
1	P	329	GLU	CA-CB-CG	-5.31	101.71	113.40
1	P	468	ALA	O-C-N	-5.30	114.21	122.70
1	P	188	GLU	O-C-N	-5.30	114.22	122.70
1	P	165	ALA	CB-CA-C	5.30	118.04	110.10
1	P	26	ILE	CA-CB-CG1	-5.29	100.94	111.00
1	P	210	ALA	CA-C-N	5.28	128.81	117.20
1	P	434	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	P	424	GLU	CA-C-O	-5.26	109.06	120.10
1	P	249	ASP	CA-CB-CG	-5.24	101.86	113.40
1	P	279	THR	CA-CB-OG1	5.24	120.01	109.00
1	P	299	ARG	CD-NE-CZ	5.23	130.92	123.60
1	P	495	PRO	CA-N-CD	-5.21	104.20	111.50
1	P	193	TRP	CD1-NE1-CE2	-5.15	104.36	109.00
1	P	22	ASN	OD1-CG-ND2	5.12	133.67	121.90
1	P	287	MET	O-C-N	-5.11	114.52	122.70
1	P	329	GLU	CG-CD-OE1	-5.11	108.08	118.30
1	P	51	GLN	CA-CB-CG	5.11	124.63	113.40
1	P	71	PRO	N-CD-CG	-5.10	95.55	103.20
1	P	170	GLY	CA-C-N	5.10	126.40	116.20
1	P	160	THR	CA-CB-CG2	5.08	119.52	112.40
1	P	189	ALA	N-CA-CB	5.08	117.22	110.10
1	P	223	TYR	O-C-N	-5.08	114.58	122.70
1	P	85	MET	CA-CB-CG	-5.06	104.70	113.30
1	P	74	ALA	CB-CA-C	-5.05	102.52	110.10
1	P	330	LEU	O-C-N	-5.04	114.64	122.70
1	P	183	ALA	N-CA-CB	5.03	117.14	110.10
1	P	316	ALA	CB-CA-C	5.03	117.64	110.10
1	P	267	ASP	CA-C-O	-5.03	109.55	120.10
1	P	88	TYR	O-C-N	5.02	130.65	121.10
1	P	299	ARG	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	128	VAL	Mainchain
1	P	150	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	P	256	ALA	Mainchain
1	P	327	THR	Mainchain
1	P	380	PRO	Mainchain
1	P	42	PRO	Mainchain
1	P	89	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	3555	0	3417	110	0
2	P	28	0	24	6	0
3	P	1	0	0	0	0
4	P	170	0	0	19	0
All	All	3754	0	3441	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (112) 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:P:423:HIS:HD2	4:P:2146:HOH:O	1.41	1.01
1:P:501:HIS:O	1:P:502:CYS:HB3	1.70	0.91
1:P:150:SER:H	1:P:153:GLN:HE21	1.17	0.86
1:P:217:ARG:O	4:P:2067:HOH:O	1.96	0.83
1:P:109:GLU:OE1	4:P:2037:HOH:O	1.96	0.83
1:P:150:SER:H	1:P:153:GLN:NE2	1.77	0.82
1:P:124:TRP:C	4:P:2039:HOH:O	2.18	0.82
1:P:449:THR:HG22	1:P:452:VAL:H	1.42	0.82
1:P:279:THR:HG23	1:P:314:ALA:HB2	1.63	0.81
1:P:143:ARG:HD3	2:P:601:NDG:H8C1	1.66	0.76
1:P:500:CYS:O	1:P:501:HIS:HB3	1.88	0.73
1:P:327:THR:HG21	1:P:361:LEU:HD11	1.71	0.72
1:P:482:ASP:HB3	1:P:485:LEU:HD22	1.73	0.70
1:P:124:TRP:O	4:P:2039:HOH:O	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:124:TRP:CA	4:P:2039:HOH:O	2.41	0.66
1:P:327:THR:CG2	1:P:361:LEU:HD11	2.26	0.66
1:P:357:ASP:OD2	4:P:2116:HOH:O	2.14	0.65
1:P:151:HIS:CD2	1:P:231:PRO:HD2	2.32	0.65
1:P:393:LYS:NZ	4:P:2132:HOH:O	2.30	0.65
1:P:400:THR:CG2	1:P:423:HIS:HE1	2.10	0.65
1:P:150:SER:N	1:P:153:GLN:HE21	1.91	0.64
1:P:102:LEU:O	4:P:2037:HOH:O	2.15	0.64
1:P:60:THR:OG1	1:P:328:HIS:HD2	1.81	0.64
1:P:502:CYS:O	1:P:502:CYS:SG	2.55	0.64
1:P:188:GLU:HG3	1:P:188:GLU:O	1.98	0.62
1:P:449:THR:HG23	1:P:451:GLU:H	1.65	0.62
1:P:177:VAL:HB	1:P:486:GLN:OE1	2.00	0.61
1:P:449:THR:CG2	1:P:451:GLU:H	2.15	0.60
1:P:210:ALA:O	1:P:211:ASP:C	2.38	0.60
1:P:357:ASP:OD1	1:P:359:SER:OG	2.17	0.59
1:P:198:GLU:CG	4:P:2069:HOH:O	2.49	0.59
1:P:327:THR:HG22	1:P:329:GLU:H	1.65	0.59
2:P:601:NDG:H6C1	2:P:602:NDG:HA	1.68	0.59
2:P:601:NDG:H6C1	2:P:602:NDG:N2	2.18	0.58
1:P:213:GLN:O	1:P:214:ARG:C	2.42	0.58
1:P:318:TRP:CB	1:P:322:ILE:HD12	2.35	0.57
1:P:24:VAL:CG1	1:P:276:VAL:HG22	2.34	0.56
1:P:297:LEU:H	1:P:297:LEU:HD23	1.71	0.55
1:P:198:GLU:HG2	4:P:2069:HOH:O	2.07	0.55
1:P:124:TRP:HA	4:P:2039:HOH:O	2.05	0.54
1:P:204:PHE:CE2	2:P:601:NDG:H8C3	2.43	0.54
1:P:111:LEU:O	1:P:116:TYR:HB2	2.06	0.54
1:P:156:CYS:HA	1:P:159:LEU:HG	1.88	0.54
1:P:129:GLY:O	4:P:2042:HOH:O	2.19	0.53
1:P:327:THR:HG23	4:P:2110:HOH:O	2.08	0.53
1:P:372:SER:HA	1:P:390:ARG:O	2.09	0.53
1:P:124:TRP:CE2	1:P:126:LEU:HB2	2.44	0.53
1:P:490:HIS:CG	1:P:493:CYS:HB3	2.44	0.52
1:P:19:ARG:CB	1:P:20:PRO:HD2	2.40	0.52
1:P:136:PRO:HG2	1:P:144:PHE:CD2	2.45	0.52
1:P:260:THR:O	1:P:261:LEU:C	2.47	0.52
1:P:279:THR:HG23	1:P:313:PRO:O	2.11	0.51
1:P:152:ASP:O	1:P:172:CYS:HB3	2.10	0.51
1:P:318:TRP:HB3	1:P:322:ILE:HD12	1.93	0.51
1:P:202:MET:HG3	1:P:260:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:163:PRO:HD3	1:P:195:PRO:HB3	1.92	0.51
1:P:93:VAL:O	1:P:96:SER:HB2	2.11	0.50
1:P:400:THR:HG21	1:P:423:HIS:HE1	1.77	0.49
1:P:199:ALA:O	1:P:200:ARG:C	2.50	0.49
1:P:70:THR:HB	1:P:71:PRO:CD	2.43	0.49
1:P:88:TYR:HB2	1:P:89:PRO:HA	1.94	0.49
1:P:22:ASN:OD1	1:P:218:PRO:HA	2.12	0.49
1:P:202:MET:SD	1:P:261:LEU:HD13	2.53	0.49
1:P:188:GLU:OE2	1:P:200:ARG:NH2	2.46	0.48
1:P:201:TYR:OH	1:P:226:HIS:HE1	1.95	0.48
1:P:20:PRO:HB2	1:P:116:TYR:OH	2.13	0.48
1:P:349:PRO:HB2	1:P:351:VAL:HG22	1.94	0.48
1:P:190:GLN:HA	1:P:191:PRO:HA	1.63	0.48
1:P:318:TRP:HB2	1:P:322:ILE:HD12	1.96	0.47
1:P:136:PRO:HG2	1:P:144:PHE:CE2	2.49	0.47
1:P:145:LEU:HD12	1:P:182:LEU:O	2.15	0.47
1:P:279:THR:CG2	1:P:313:PRO:O	2.63	0.47
1:P:327:THR:CG2	4:P:2110:HOH:O	2.63	0.46
1:P:128:VAL:HB	4:P:2041:HOH:O	2.15	0.46
1:P:428:LEU:H	1:P:440:ASN:ND2	2.13	0.46
1:P:204:PHE:CD2	2:P:601:NDG:H8C3	2.50	0.46
1:P:396:ALA:HB2	1:P:459:LEU:HD13	1.97	0.46
1:P:261:LEU:O	1:P:265:ILE:HG13	2.14	0.46
1:P:75:ALA:HB1	1:P:334:LEU:HD13	1.97	0.46
1:P:123:LYS:HD2	1:P:150:SER:HA	1.97	0.45
1:P:70:THR:N	1:P:71:PRO:HD2	2.30	0.45
1:P:43:SER:OG	1:P:244:ARG:HG3	2.17	0.45
1:P:400:THR:HB	1:P:423:HIS:CE1	2.52	0.45
1:P:197:LEU:O	1:P:198:GLU:C	2.56	0.45
1:P:440:ASN:ND2	1:P:442:LEU:H	2.14	0.45
1:P:268:LEU:HB2	1:P:270:LEU:HG	1.99	0.45
1:P:263:THR:O	1:P:264:ALA:C	2.52	0.45
1:P:179:ILE:O	1:P:191:PRO:HA	2.17	0.44
1:P:241:ARG:CB	1:P:252:MET:HE1	2.47	0.44
1:P:242:SER:HB3	1:P:252:MET:HE2	1.98	0.44
1:P:81:LEU:HA	1:P:82:PRO:HD3	1.82	0.44
1:P:460:GLN:CD	4:P:2161:HOH:O	2.55	0.44
1:P:442:LEU:O	1:P:443:GLY:C	2.56	0.43
1:P:442:LEU:HD12	1:P:442:LEU:HA	1.82	0.43
1:P:198:GLU:O	1:P:201:TYR:N	2.52	0.43
1:P:318:TRP:CD2	1:P:321:HIS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:500:CYS:O	1:P:501:HIS:CB	2.62	0.43
1:P:190:GLN:HG2	1:P:501:HIS:HA	2.01	0.43
1:P:266:GLY:O	1:P:267:ASP:C	2.57	0.42
1:P:62:PHE:CE1	1:P:279:THR:HG21	2.54	0.42
1:P:24:VAL:HG13	1:P:276:VAL:HG22	2.01	0.42
1:P:227:HIS:HA	4:P:2072:HOH:O	2.18	0.42
1:P:142:HIS:HB3	2:P:602:NDG:H8C3	2.01	0.42
1:P:198:GLU:HG3	4:P:2069:HOH:O	2.15	0.42
1:P:28:ALA:HB2	1:P:254:LEU:HD11	2.02	0.41
1:P:112:ALA:O	1:P:115:GLY:N	2.47	0.41
1:P:177:VAL:HG22	1:P:500:CYS:HB2	2.03	0.41
1:P:278:PHE:O	1:P:314:ALA:HA	2.21	0.41
1:P:183:ALA:O	1:P:184:ASN:C	2.59	0.41
1:P:124:TRP:O	1:P:125:HIS:C	2.59	0.40
1:P:23:ILE:HD13	1:P:340:LEU:HD22	2.03	0.40
1:P:213:GLN:O	1:P:216:ASP:N	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	476/489 (97%)	440 (92%)	32 (7%)	4 (1%)	24 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	493	CYS
1	P	502	CYS
1	P	172	CYS
1	P	501	HIS

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	P	370/384 (96%)	326 (88%)	44 (12%)	6	12

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	27	PHE
1	P	52	LEU
1	P	85	MET
1	P	96	SER
1	P	103	GLU
1	P	111	LEU
1	P	149	TYR
1	P	161	CYS
1	P	169	ASP
1	P	177	VAL
1	P	179	ILE
1	P	185	LEU
1	P	188	GLU
1	P	217	ARG
1	P	236	GLN
1	P	237	SER
1	P	240	GLU
1	P	254	LEU
1	P	261	LEU
1	P	262	MET
1	P	272	GLU
1	P	279	THR
1	P	282	ASN
1	P	290	SER
1	P	327	THR
1	P	334	LEU
1	P	337	LEU
1	P	343	LEU
1	P	351	VAL
1	P	352	THR

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Mol	Chain	Res	Type
1	P	367	LYS
1	P	368	SER
1	P	377	PRO
1	P	400	THR
1	P	426	LEU
1	P	440	ASN
1	P	442	LEU
1	P	449	THR
1	P	451	GLU
1	P	471	THR
1	P	485	LEU
1	P	501	HIS
1	P	502	CYS
1	P	503	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	153	GLN
1	P	226	HIS
1	P	328	HIS
1	P	423	HIS
1	P	440	ASN
1	P	465	GLN
1	P	490	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	DDZ	P	69	1,3	2,6,7	1.10	0	1,7,9	5.20	1 (100%)

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
1	DDZ	P	69	1,3	-	0/0/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	69	DDZ	C-CA-N	5.20	120.41	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDG	P	601	1,2	14,14,15	2.07	5 (35%)	15,19,21	4.12	11 (73%)
2	NDG	P	602	2	14,14,15	1.37	2 (14%)	15,19,21	2.87	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	P	601	1,2	-	0/6/23/26	0/1/1/1
2	NDG	P	602	2	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	602	NDG	O7-C7	-3.46	1.15	1.23
2	P	601	NDG	O7-C7	-3.32	1.15	1.23
2	P	601	NDG	O4-C4	-3.15	1.35	1.43
2	P	601	NDG	O-C5	-2.54	1.37	1.43
2	P	601	NDG	C4-C5	2.16	1.57	1.53
2	P	602	NDG	C1-C2	2.31	1.55	1.52
2	P	601	NDG	C2-N2	4.34	1.54	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	601	NDG	O7-C7-N2	-5.62	110.41	121.86
2	P	601	NDG	C2-N2-C7	-4.46	117.31	123.04
2	P	601	NDG	O4-C4-C5	-4.31	97.82	109.24
2	P	601	NDG	C3-C2-N2	-4.08	100.78	110.56
2	P	601	NDG	C3-C4-C5	-4.08	103.08	110.20
2	P	601	NDG	C6-C5-C4	-3.05	105.49	113.02
2	P	602	NDG	O3-C3-C2	-2.90	103.36	109.11
2	P	602	NDG	C2-N2-C7	-2.61	119.68	123.04
2	P	601	NDG	O3-C3-C2	2.14	113.36	109.11
2	P	601	NDG	O-C5-C6	2.69	113.18	107.35
2	P	601	NDG	C1-O-C5	5.68	119.46	112.25
2	P	601	NDG	O4-C4-C3	6.66	125.34	110.34
2	P	601	NDG	C8-C7-N2	6.69	128.91	116.11
2	P	602	NDG	C1-O-C5	9.64	124.48	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	601	NDG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	602	NDG	3	0

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	P	480/489 (98%)	-0.47	3 (0%) 90 91	18, 38, 64, 92	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	26	ILE	2.7
1	P	27	PHE	2.2
1	P	25	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	DDZ	P	69	7/8	0.96	0.19	-	28,28,32,33	0

6.3 Carbohydrates

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NDG	P	601	14/15	0.96	0.17	1.12	54,60,72,80	0
2	NDG	P	602	14/15	0.84	0.25	-	86,94,107,111	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	P	603	1/1	0.98	0.26	1.53	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.