



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:06 PM GMT

PDB ID : 1E2S  
Title : CRYSTAL STRUCTURE OF AN ARYLSULFATASE A MUTANT C69A  
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Deposited on : 2000-05-24  
Resolution : 2.35 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](mailto: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.

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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

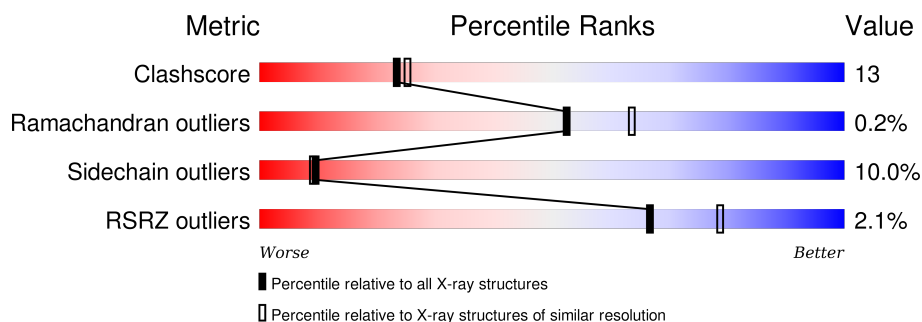
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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  $\geq 3$ , 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 5 unique types of molecules in this entry. The entry contains 3773 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
			3553	2270	603	657	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	69	ALA	CYS	ENGINEERED MUTATION	UNP P15289

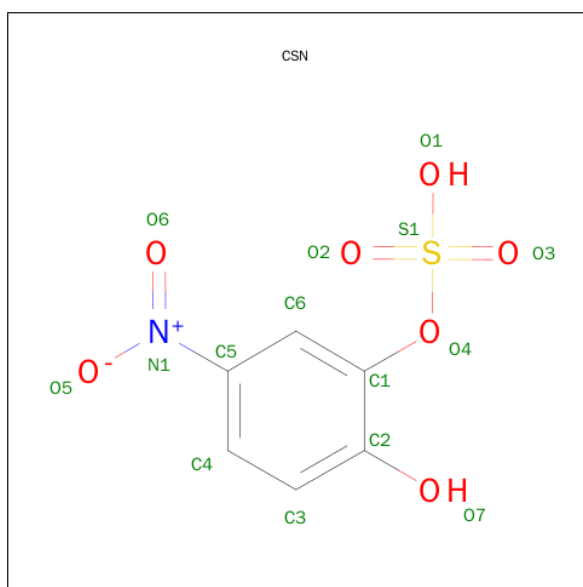
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is N,4-DIHYDROXY-N-OXO-3-(SULFOOXY)BENZENAMINIUM (three-letter code: CSN) (formula: C<sub>6</sub>H<sub>5</sub>NO<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	P	1	Total	C	N	O	S	0	1
			25	12	2	10	1		

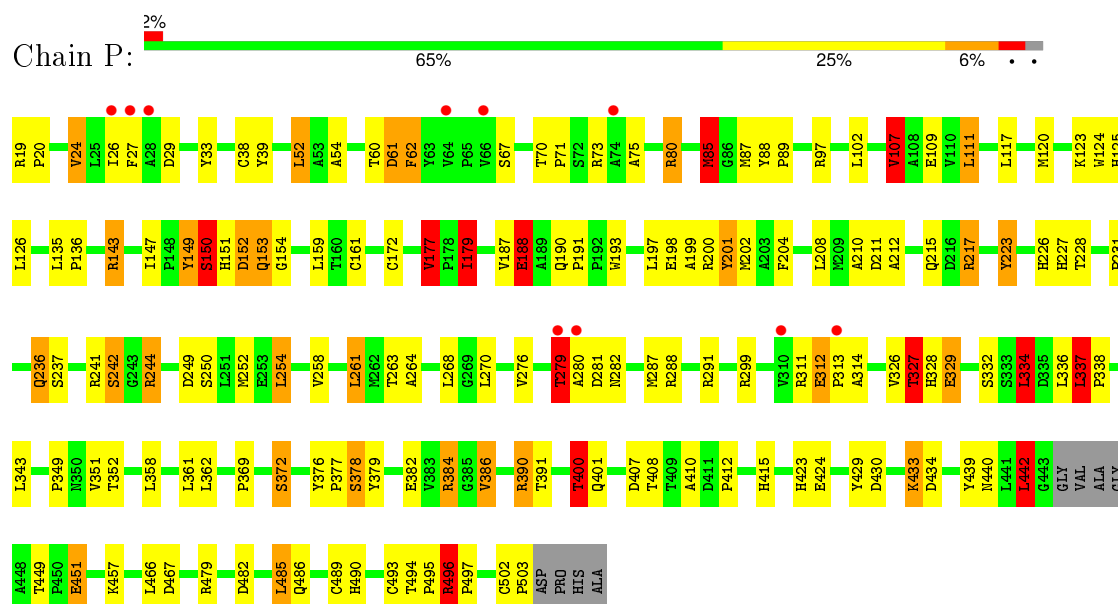
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	166	Total	O	0	0
			166	166		

### 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, $\alpha$ , $\beta$ , $\gamma$	131.80Å 131.80Å 192.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.35 38.81 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-2.35) 99.3 (38.81-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.03 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.191 , 0.236 0.165 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.5	EDS
Estimated twinning fraction	0.013 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 <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 35240 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, CSN, 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	0.93	2/3660 (0.1%)	1.89	97/5003 (1.9%)

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	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	503	PRO	N-CD	6.04	1.56	1.47
1	P	150	SER	CA-CB	5.01	1.60	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	291	ARG	NE-CZ-NH1	18.46	129.53	120.30
1	P	291	ARG	NE-CZ-NH2	-17.82	111.39	120.30
1	P	80	ARG	NE-CZ-NH2	14.62	127.61	120.30
1	P	33	TYR	CB-CG-CD1	-14.46	112.33	121.00
1	P	299	ARG	NE-CZ-NH1	-14.05	113.28	120.30
1	P	179	ILE	CA-CB-CG2	12.21	135.32	110.90
1	P	73	ARG	NE-CZ-NH1	-11.64	114.48	120.30
1	P	329	GLU	OE1-CD-OE2	10.65	136.08	123.30
1	P	281	ASP	CB-CG-OD1	10.40	127.66	118.30
1	P	73	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	P	496	ARG	NE-CZ-NH2	10.22	125.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	80	ARG	NE-CZ-NH1	-10.13	115.23	120.30
1	P	33	TYR	CB-CG-CD2	9.55	126.73	121.00
1	P	244	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	P	299	ARG	NH1-CZ-NH2	8.95	129.24	119.40
1	P	177	VAL	N-CA-CB	-8.85	92.04	111.50
1	P	384	ARG	CD-NE-CZ	-8.75	111.35	123.60
1	P	390	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	P	311	ARG	CD-NE-CZ	8.23	135.12	123.60
1	P	489	CYS	CA-CB-SG	-8.09	99.43	114.00
1	P	384	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	P	479	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	P	152	ASP	CB-CG-OD2	7.76	125.28	118.30
1	P	279	THR	CA-CB-OG1	7.52	124.78	109.00
1	P	29	ASP	CB-CG-OD2	7.38	124.94	118.30
1	P	429	TYR	CB-CG-CD1	-7.18	116.69	121.00
1	P	97	ARG	CD-NE-CZ	7.10	133.54	123.60
1	P	291	ARG	CD-NE-CZ	7.06	133.49	123.60
1	P	337	LEU	CA-CB-CG	6.98	131.35	115.30
1	P	150	SER	N-CA-CB	6.96	120.94	110.50
1	P	494	THR	CA-C-O	-6.77	105.89	120.10
1	P	327	THR	CB-CA-C	-6.74	93.41	111.60
1	P	390	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	P	439	TYR	CB-CG-CD2	6.61	124.97	121.00
1	P	287	MET	N-CA-CB	-6.55	98.81	110.60
1	P	39	TYR	CG-CD1-CE1	-6.48	116.11	121.30
1	P	386	VAL	CA-CB-CG1	-6.44	101.24	110.90
1	P	85	MET	CA-CB-CG	-6.43	102.37	113.30
1	P	107	VAL	CB-CA-C	-6.39	99.25	111.40
1	P	38	CYS	CA-CB-SG	6.36	125.44	114.00
1	P	143	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	P	329	GLU	CA-CB-CG	-6.29	99.57	113.40
1	P	467	ASP	CB-CG-OD1	6.27	123.94	118.30
1	P	489	CYS	C-N-CA	6.26	137.36	121.70
1	P	496	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	P	242	SER	CA-C-N	6.21	128.63	116.20
1	P	312	GLU	CG-CD-OE1	6.19	130.69	118.30
1	P	193	TRP	CB-CG-CD1	6.19	135.05	127.00
1	P	279	THR	N-CA-CB	6.18	122.05	110.30
1	P	378	SER	CB-CA-C	-6.16	98.39	110.10
1	P	391	THR	OG1-CB-CG2	-6.11	95.94	110.00
1	P	62	PHE	O-C-N	-6.06	113.01	122.70
1	P	408	THR	N-CA-CB	6.03	121.75	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	61	ASP	CB-CG-OD1	5.97	123.67	118.30
1	P	188	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	P	120	MET	CG-SD-CE	-5.93	90.71	100.20
1	P	386	VAL	CG1-CB-CG2	-5.92	101.43	110.90
1	P	52	LEU	CA-CB-CG	5.88	128.81	115.30
1	P	73	ARG	CD-NE-CZ	5.86	131.80	123.60
1	P	424	GLU	CA-C-O	-5.80	107.93	120.10
1	P	244	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	P	439	TYR	CB-CG-CD1	-5.71	117.57	121.00
1	P	494	THR	O-C-N	5.71	131.96	121.10
1	P	250	SER	N-CA-CB	-5.64	102.04	110.50
1	P	299	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	P	177	VAL	CA-CB-CG1	5.59	119.28	110.90
1	P	434	ASP	CB-CG-OD1	5.59	123.33	118.30
1	P	288	ARG	CG-CD-NE	-5.56	100.12	111.80
1	P	254	LEU	CB-CA-C	-5.55	99.66	110.20
1	P	372	SER	CA-CB-OG	-5.55	96.22	111.20
1	P	249	ASP	CB-CG-OD1	5.51	123.26	118.30
1	P	217	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	P	201	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	P	111	LEU	CA-CB-CG	5.40	127.72	115.30
1	P	187	VAL	CG1-CB-CG2	5.38	119.52	110.90
1	P	391	THR	N-CA-CB	5.38	120.53	110.30
1	P	496	ARG	CA-C-O	-5.34	108.88	120.10
1	P	401	GLN	N-CA-CB	-5.33	101.00	110.60
1	P	334	LEU	CB-CG-CD1	5.32	120.04	111.00
1	P	193	TRP	CB-CG-CD2	-5.30	119.71	126.60
1	P	400	THR	N-CA-CB	-5.28	100.26	110.30
1	P	495	PRO	CA-N-CD	-5.27	104.12	111.50
1	P	193	TRP	CD1-NE1-CE2	-5.23	104.29	109.00
1	P	242	SER	C-N-CA	-5.21	111.35	122.30
1	P	497	PRO	CA-N-CD	-5.21	104.20	111.50
1	P	279	THR	CB-CA-C	-5.19	97.60	111.60
1	P	400	THR	CA-CB-OG1	5.18	119.88	109.00
1	P	201	TYR	CB-CG-CD1	5.17	124.10	121.00
1	P	223	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	P	208	LEU	CA-CB-CG	5.11	127.06	115.30
1	P	67	SER	CB-CA-C	5.11	119.81	110.10
1	P	442	LEU	O-C-N	-5.11	114.52	123.20
1	P	326	VAL	CA-C-N	5.10	128.41	117.20
1	P	223	TYR	CB-CG-CD1	5.05	124.03	121.00
1	P	153	GLN	O-C-N	-5.04	114.63	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	299	ARG	N-CA-CB	-5.02	101.57	110.60
1	P	496	ARG	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	107	VAL	Mainchain
1	P	223	TYR	Mainchain
1	P	241	ARG	Mainchain
1	P	327	THR	Mainchain
1	P	442	LEU	Mainchain
1	P	54	ALA	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	3553	0	3421	92	1
2	P	1	0	0	0	0
3	P	28	0	25	4	0
4	P	25	0	6	2	0
5	P	166	0	0	17	0
All	All	3773	0	3452	94	1

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 13.

All (94) 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	5:P:2140:HOH:O	1.50	0.93
1:P:109:GLU:OE2	5:P:2038:HOH:O	1.92	0.87
1:P:109:GLU:CD	5:P:2038:HOH:O	2.16	0.84
1:P:386:VAL:HG11	1:P:466:LEU:HD23	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:109:GLU:OE1	5:P:2038:HOH:O	1.99	0.80
1:P:327:THR:HG23	5:P:2107:HOH:O	1.83	0.78
1:P:204:PHE:CE2	3:P:601:NDG:H8C3	2.26	0.70
1:P:407:ASP:OD1	5:P:2134:HOH:O	2.10	0.69
1:P:19:ARG:N	1:P:20:PRO:HD2	2.09	0.67
1:P:150:SER:H	1:P:153:GLN:HE21	1.42	0.67
1:P:198:GLU:HB3	5:P:2063:HOH:O	1.95	0.65
1:P:198:GLU:CG	5:P:2070:HOH:O	2.45	0.65
1:P:358:LEU:HD22	1:P:369:PRO:HD2	1.78	0.65
1:P:242:SER:N	1:P:252:MET:HE1	2.11	0.65
1:P:386:VAL:HG11	1:P:466:LEU:CD2	2.27	0.64
1:P:198:GLU:HG3	5:P:2070:HOH:O	1.98	0.63
1:P:24:VAL:HG13	1:P:276:VAL:HG22	1.79	0.63
1:P:62:PHE:CE1	1:P:279:THR:HG21	2.34	0.62
1:P:376:TYR:CZ	1:P:386:VAL:HG12	2.35	0.61
1:P:177:VAL:HB	1:P:486:GLN:OE1	2.01	0.60
1:P:102:LEU:O	5:P:2034:HOH:O	2.17	0.60
1:P:143:ARG:HD3	3:P:601:NDG:H8C1	1.84	0.59
1:P:327:THR:HG22	1:P:329:GLU:H	1.68	0.59
1:P:123:LYS:HZ1	1:P:150:SER:HB3	1.68	0.58
1:P:24:VAL:CG1	1:P:276:VAL:HG22	2.34	0.57
1:P:386:VAL:CG1	1:P:466:LEU:HD23	2.33	0.57
1:P:407:ASP:CB	5:P:2134:HOH:O	2.54	0.56
1:P:149:TYR:HB2	1:P:153:GLN:NE2	2.21	0.56
1:P:204:PHE:HE2	3:P:601:NDG:H8C3	1.72	0.55
1:P:204:PHE:CD2	3:P:601:NDG:H8C3	2.42	0.55
1:P:279:THR:HG23	1:P:314:ALA:HB2	1.88	0.54
1:P:159:LEU:HD21	1:P:191:PRO:HG3	1.90	0.54
1:P:279:THR:HG23	1:P:313:PRO:O	2.07	0.53
1:P:201:TYR:OH	1:P:226:HIS:HE1	1.90	0.53
1:P:117:LEU:HD23	1:P:212:ALA:HB2	1.90	0.53
1:P:400:THR:CG2	1:P:423:HIS:HE1	2.22	0.52
1:P:123:LYS:NZ	1:P:150:SER:HB3	2.25	0.52
1:P:150:SER:H	1:P:153:GLN:NE2	2.05	0.51
1:P:215:GLN:HB2	1:P:217:ARG:HG2	1.93	0.51
1:P:378:SER:HB2	1:P:379:TYR:CD1	2.47	0.50
1:P:151:HIS:CD2	1:P:231:PRO:HD2	2.47	0.50
1:P:449:THR:HG22	1:P:451:GLU:H	1.76	0.50
1:P:378:SER:HB2	1:P:379:TYR:HD1	1.77	0.50
1:P:75:ALA:HB1	1:P:334:LEU:HD13	1.94	0.50
1:P:85:MET:HG3	1:P:87:MET:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:124:TRP:CE2	1:P:126:LEU:HB2	2.47	0.49
1:P:60:THR:OG1	1:P:328:HIS:HD2	1.96	0.49
1:P:202:MET:SD	1:P:261:LEU:HD13	2.53	0.48
1:P:337:LEU:HB3	1:P:338:PRO:CD	2.42	0.48
1:P:407:ASP:CG	5:P:2134:HOH:O	2.49	0.48
1:P:502:CYS:O	1:P:502:CYS:SG	2.70	0.48
1:P:26:ILE:HD13	1:P:258:VAL:HG22	1.95	0.48
1:P:415:HIS:CD2	5:P:2136:HOH:O	2.68	0.47
1:P:264:ALA:O	1:P:268:LEU:HG	2.15	0.47
1:P:312:GLU:HB3	1:P:313:PRO:HD2	1.97	0.47
1:P:236:GLN:O	1:P:236:GLN:HG3	2.15	0.47
1:P:190:GLN:HA	1:P:191:PRO:HA	1.68	0.46
1:P:152:ASP:O	1:P:172:CYS:HB3	2.16	0.46
1:P:154:GLY:O	1:P:172:CYS:HB2	2.16	0.46
1:P:150:SER:N	1:P:153:GLN:HE21	2.11	0.46
1:P:70:THR:N	1:P:71:PRO:HD2	2.31	0.45
1:P:400:THR:HG23	5:P:2138:HOH:O	2.16	0.45
1:P:440:ASN:ND2	1:P:442:LEU:H	2.15	0.45
1:P:449:THR:HG22	1:P:451:GLU:N	2.32	0.45
1:P:279:THR:CG2	1:P:313:PRO:O	2.65	0.44
1:P:80:ARG:HB2	1:P:85:MET:HE1	1.99	0.44
1:P:332:SER:OG	1:P:334:LEU:HB2	2.18	0.44
1:P:482:ASP:HB3	1:P:485:LEU:HD22	1.99	0.44
1:P:415:HIS:HD2	5:P:2136:HOH:O	1.99	0.44
1:P:210:ALA:O	1:P:211:ASP:C	2.54	0.43
1:P:372:SER:HA	1:P:390:ARG:O	2.18	0.43
1:P:199:ALA:O	1:P:200:ARG:C	2.54	0.43
1:P:349:PRO:HB2	1:P:351:VAL:HG22	1.99	0.43
1:P:268:LEU:HB2	1:P:270:LEU:HG	2.01	0.43
1:P:268:LEU:HD23	1:P:268:LEU:N	2.33	0.43
1:P:135:LEU:HB3	1:P:136:PRO:HD2	2.00	0.43
1:P:159:LEU:HD21	1:P:191:PRO:CG	2.50	0.42
1:P:198:GLU:OE1	5:P:2064:HOH:O	2.22	0.42
1:P:279:THR:HG22	1:P:280:ALA:H	1.83	0.42
1:P:263:THR:O	1:P:264:ALA:C	2.56	0.42
1:P:337:LEU:CB	1:P:338:PRO:CD	2.97	0.42
1:P:227:HIS:HA	1:P:228:THR:HA	1.75	0.42
1:P:410:ALA:O	1:P:412:PRO:HD3	2.20	0.42
1:P:188:GLU:HG3	1:P:188:GLU:O	2.19	0.42
1:P:327:THR:HG21	1:P:361:LEU:HD11	2.02	0.41
1:P:123:LYS:HD2	1:P:150:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:496:ARG:NH1	5:P:2164:HOH:O	2.53	0.41
1:P:384:ARG:HD3	1:P:384:ARG:HH11	1.49	0.41
1:P:430:ASP:OD2	1:P:433:LYS:HE2	2.20	0.41
1:P:88:TYR:HB2	1:P:89:PRO:HA	2.02	0.41
1:P:244:ARG:O	1:P:244:ARG:HG2	2.21	0.40
1:P:147:ILE:HD13	1:P:179:ILE:HG23	2.02	0.40

All (1) 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:P:490:HIS:NE2	1:P:490:HIS:NE2[16_554]	2.10	0.10

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	477/489 (98%)	446 (94%)	30 (6%)	1 (0%)	52 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	493	CYS

### 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	369/384 (96%)	332 (90%)	37 (10%)	9 9

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	24	VAL
1	P	27	PHE
1	P	52	LEU
1	P	61	ASP
1	P	85	MET
1	P	107	VAL
1	P	111	LEU
1	P	125	HIS
1	P	149	TYR
1	P	150	SER
1	P	161	CYS
1	P	177	VAL
1	P	179	ILE
1	P	188	GLU
1	P	197	LEU
1	P	236	GLN
1	P	237	SER
1	P	254	LEU
1	P	261	LEU
1	P	279	THR
1	P	282	ASN
1	P	327	THR
1	P	334	LEU
1	P	336	LEU
1	P	337	LEU
1	P	343	LEU
1	P	352	THR
1	P	362	LEU
1	P	377	PRO
1	P	382	GLU
1	P	400	THR
1	P	433	LYS
1	P	442	LEU
1	P	451	GLU
1	P	457	LYS
1	P	485	LEU
1	P	496	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) 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

### 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 ⓘ

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$
3	NDG	P	601	1,3	14,14,15	1.67	4 (28%)	15,19,21	3.58	9 (60%)
3	NDG	P	602	3	14,14,15	1.36	2 (14%)	15,19,21	2.28	5 (33%)

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	NDG	P	601	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	P	602	3	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	602	NDG	O7-C7	-3.25	1.15	1.23
3	P	601	NDG	O7-C7	-3.21	1.15	1.23
3	P	601	NDG	O-C5	-2.48	1.38	1.43
3	P	601	NDG	O4-C4	-2.20	1.37	1.43
3	P	602	NDG	C2-N2	2.49	1.50	1.46
3	P	601	NDG	C2-N2	2.91	1.51	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	601	NDG	O7-C7-N2	-6.41	108.80	121.86
3	P	601	NDG	O4-C4-C5	-4.19	98.14	109.24
3	P	602	NDG	C2-N2-C7	-3.81	118.14	123.04
3	P	601	NDG	C3-C2-N2	-3.16	103.00	110.56
3	P	602	NDG	O3-C3-C2	-2.65	103.85	109.11
3	P	601	NDG	C3-C4-C5	-2.37	106.07	110.20
3	P	601	NDG	C6-C5-C4	-2.19	107.62	113.02
3	P	602	NDG	O4-C4-C3	-2.02	105.78	110.34
3	P	602	NDG	C3-C4-C5	2.96	115.36	110.20
3	P	601	NDG	O3-C3-C2	2.97	114.99	109.11
3	P	601	NDG	C1-O-C5	3.83	117.11	112.25
3	P	602	NDG	C1-O-C5	6.20	120.11	112.25
3	P	601	NDG	O4-C4-C3	6.32	124.57	110.34
3	P	601	NDG	C8-C7-N2	6.45	128.45	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	601	NDG	4	0

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
4	CSN	P	701[A]	-	13,15,15	1.22	2 (15%)	16,22,22	3.93	9 (56%)
4	CSN	P	701[B]	-	13,15,15	1.23	1 (7%)	16,22,22	2.58	9 (56%)

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
4	CSN	P	701[A]	-	-	1/9/9/9	0/1/1/1
4	CSN	P	701[B]	-	-	0/9/9/9	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	701[B]	CSN	O7-C2	-3.65	1.28	1.36
4	P	701[A]	CSN	O7-C2	-2.97	1.30	1.36
4	P	701[A]	CSN	O4-C1	-2.23	1.37	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	701[A]	CSN	C6-C5-N1	-6.56	113.05	118.80
4	P	701[A]	CSN	C3-C2-C1	-5.42	112.57	119.50
4	P	701[B]	CSN	C6-C5-N1	-4.65	114.72	118.80
4	P	701[B]	CSN	C5-C6-C1	-3.47	114.83	119.14
4	P	701[A]	CSN	O4-C1-C2	-2.43	115.12	118.00
4	P	701[B]	CSN	O4-C1-C6	-2.30	114.86	118.70
4	P	701[B]	CSN	C3-C2-C1	-2.07	116.85	119.50
4	P	701[B]	CSN	O1-S1-O2	2.02	116.14	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	701[A]	CSN	O1-S1-O2	2.02	116.14	108.56
4	P	701[B]	CSN	C4-C5-N1	2.54	121.53	119.48
4	P	701[B]	CSN	C4-C5-C6	2.63	123.72	120.07
4	P	701[A]	CSN	C4-C3-C2	2.66	123.22	120.49
4	P	701[A]	CSN	O6-N1-C5	2.96	124.21	118.89
4	P	701[A]	CSN	O7-C2-C3	3.06	127.74	119.35
4	P	701[B]	CSN	O7-C2-C1	3.98	129.25	120.10
4	P	701[B]	CSN	C6-C1-C2	4.41	124.78	120.04
4	P	701[A]	CSN	C6-C1-C2	5.18	125.61	120.04
4	P	701[A]	CSN	C4-C5-N1	10.53	127.97	119.48

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	701[A]	CSN	S1-O4-C1-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	701[A]	CSN	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	P	481/489 (98%)	-0.20	10 (2%) 67 79	23, 40, 65, 86	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	27	PHE	3.0
1	P	279	THR	2.7
1	P	280	ALA	2.6
1	P	64	VAL	2.6
1	P	310	VAL	2.4
1	P	313	PRO	2.3
1	P	26	ILE	2.2
1	P	74	ALA	2.2
1	P	28	ALA	2.2
1	P	66	VAL	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NDG	P	601	14/15	0.95	0.12	0.37	51,63,72,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NDG	P	602	14/15	0.77	0.22	-	82,89,95,98	0

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	CSN	P	701[B]	15/15	0.94	0.18	0.82	53,64,72,73	10
4	CSN	P	701[A]	15/15	0.94	0.18	-0.15	53,64,69,72	10
2	MG	P	600	1/1	0.98	0.20	-0.38	34,34,34,34	0

## 6.5 Other polymers

There are no such residues in this entry.