



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:07 pm BST

PDB ID : 1UP8  
Title : Recombinant vanadium-dependent bromoperoxidase from red algae *Corallina pilulifera*  
Authors : Garcia-Rodriguez, E.; Isupov, M.; Ohshiro, T.; Izumi, Y.; Littlechild, J.A.  
Deposited on : 2003-09-29  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

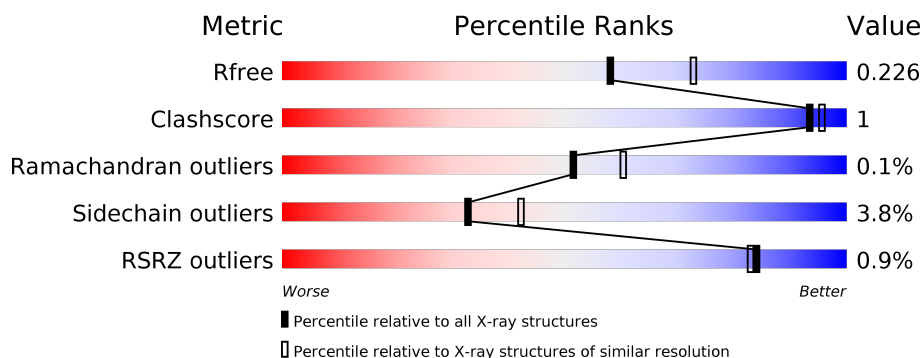
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	598	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	598	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
1	C	598	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	598	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20832 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.

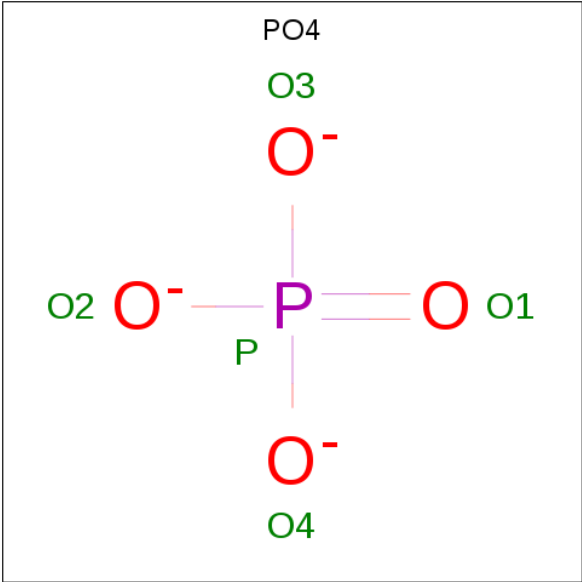
- Molecule 1 is a protein called VANADIUM-DEPENDENT BROMOPEROXIDASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4605	2926	769	903	7			
1	B	597	Total	C	N	O	S	0	0	0
			4605	2926	769	903	7			
1	C	597	Total	C	N	O	S	0	0	0
			4605	2926	769	903	7			
1	D	597	Total	C	N	O	S	0	0	0
			4605	2926	769	903	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	ALA	PRO	SEE REMARK 999	UNP O81959
B	421	ALA	PRO	SEE REMARK 999	UNP O81959
C	421	ALA	PRO	SEE REMARK 999	UNP O81959
D	421	ALA	PRO	SEE REMARK 999	UNP O81959

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

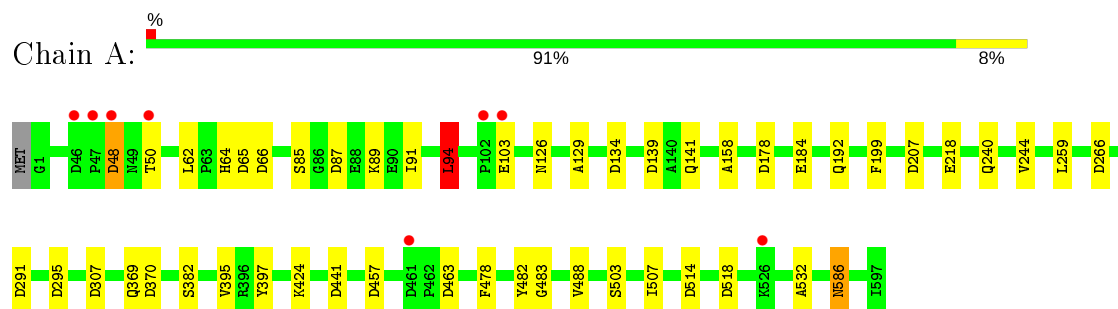
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	558	Total	O	0	0
			558	558		
4	B	606	Total	O	0	0
			606	606		
4	C	566	Total	O	0	0
			566	566		
4	D	598	Total	O	0	0
			598	598		

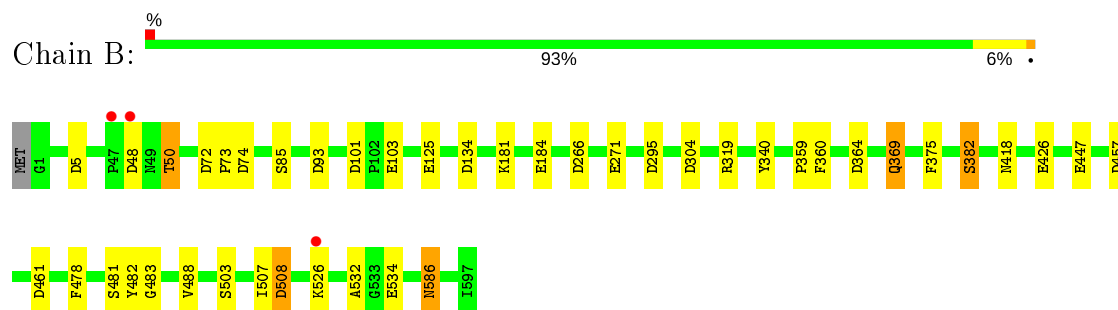
### 3 Residue-property plots [i](#)

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

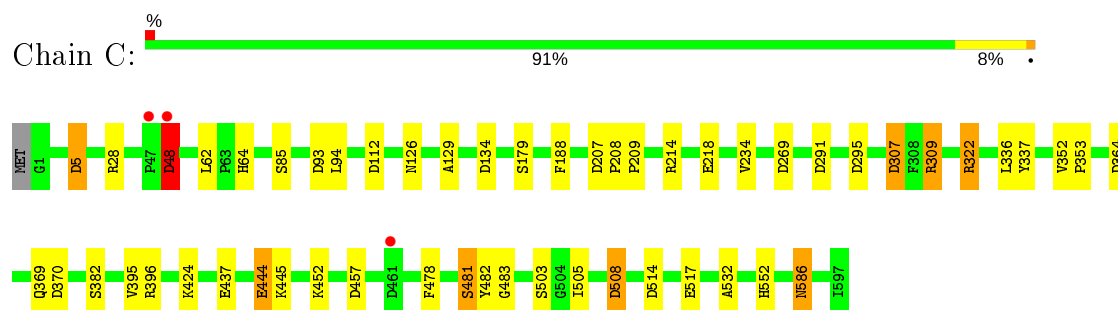
#### • Molecule 1: VANADIUM-DEPENDENT BROMOPEROXIDASE 1



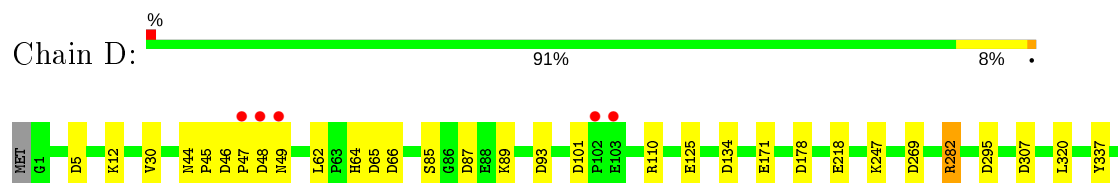
#### • Molecule 1: VANADIUM-DEPENDENT BROMOPEROXIDASE 1

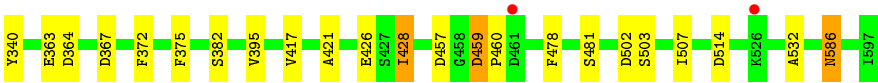


#### • Molecule 1: VANADIUM-DEPENDENT BROMOPEROXIDASE 1



#### • Molecule 1: VANADIUM-DEPENDENT BROMOPEROXIDASE 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.95Å 185.95Å 180.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.00 – 2.20 21.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (22.00-2.20) 92.6 (21.97-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.168 , 0.223 0.172 , 0.226	Depositor DCC
$R_{free}$ test set	8213 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, PO4

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	0.75	0/4705	0.82	17/6395 (0.3%)
1	B	0.77	0/4705	0.83	12/6395 (0.2%)
1	C	0.75	0/4705	0.84	20/6395 (0.3%)
1	D	0.77	0/4705	0.85	16/6395 (0.3%)
All	All	0.76	0/18820	0.84	65/25580 (0.3%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	C	322	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	C	322	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	D	282	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	461	ASP	CB-CG-OD2	7.26	124.84	118.30
1	D	459	ASP	CB-CG-OD2	7.18	124.77	118.30
1	C	295	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	65	ASP	CB-CG-OD2	6.74	124.36	118.30
1	C	457	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	266	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	291	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	295	ASP	CB-CG-OD2	6.53	124.18	118.30
1	D	514	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	518	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	457	ASP	CB-CG-OD2	6.34	124.00	118.30
1	C	514	ASP	CB-CG-OD2	6.27	123.94	118.30
1	D	65	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	307	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	214	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	364	ASP	CB-CG-OD2	6.08	123.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	ASP	CB-CG-OD2	6.04	123.74	118.30
1	D	134	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	266	ASP	CB-CG-OD2	5.79	123.52	118.30
1	D	101	ASP	CB-CG-OD2	5.77	123.49	118.30
1	D	364	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	93	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	94	LEU	CA-CB-CG	5.68	128.36	115.30
1	C	134	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	457	ASP	CB-CG-OD2	5.65	123.38	118.30
1	C	112	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	139	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	134	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	207	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	28	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	48	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	508	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	28	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	457	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	5	ASP	CB-CG-OD2	5.39	123.16	118.30
1	D	295	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	134	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	110	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	93	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	319	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	B	101	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	48	ASP	CB-CG-OD2	5.26	123.03	118.30
1	D	307	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	441	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	463	ASP	CB-CG-OD2	5.22	122.99	118.30
1	C	309	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	307	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	367	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	87	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	364	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	93	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	269	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	514	ASP	CB-CG-OD2	5.11	122.89	118.30
1	D	502	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	87	ASP	CB-CG-OD2	5.09	122.89	118.30
1	C	291	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	304	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	207	ASP	CB-CG-OD2	5.07	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	74	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	508	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	66	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4605	0	4492	13	0
1	B	4605	0	4492	11	0
1	C	4605	0	4492	17	0
1	D	4605	0	4492	13	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	558	0	0	2	0
4	B	606	0	0	0	0
4	C	566	0	0	2	0
4	D	598	0	0	1	0
All	All	20832	0	17968	51	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 1.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
4:A:2415:HOH:O	1:B:382:SER:HB2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:SER:HB2	1:A:532:ALA:HB2	1.83	0.60
1:C:307:ASP:OD1	1:C:309:ARG:HD3	2.04	0.56
1:A:259:LEU:HD12	1:A:259:LEU:N	2.21	0.55
1:C:5:ASP:HB3	4:C:2010:HOH:O	2.06	0.55
1:B:586:ASN:HD22	1:B:586:ASN:C	2.10	0.54
1:D:421:ALA:HB1	1:D:426:GLU:HG3	1.91	0.52
1:D:282:ARG:HG2	1:D:320:LEU:N	2.27	0.49
1:C:322:ARG:NH2	1:C:517:GLU:O	2.44	0.49
1:C:586:ASN:HD22	1:C:586:ASN:C	2.15	0.49
1:C:370:ASP:HB3	1:D:125:GLU:HG2	1.95	0.48
1:A:370:ASP:HB3	1:B:125:GLU:HG2	1.96	0.47
1:C:126:ASN:HB3	1:C:129:ALA:HB2	1.97	0.47
1:A:482:TYR:HA	1:A:483:GLY:HA2	1.78	0.47
1:A:192:GLN:NE2	4:A:2252:HOH:O	2.49	0.46
1:C:482:TYR:HA	1:C:483:GLY:HA2	1.74	0.46
1:D:46:ASP:HA	1:D:47:PRO:HD3	1.68	0.46
1:D:269:ASP:CG	1:D:282:ARG:HH22	2.19	0.45
1:D:586:ASN:C	1:D:586:ASN:HD22	2.19	0.45
1:D:44:ASN:OD1	1:D:45:PRO:HD2	2.16	0.45
1:B:50:THR:O	1:B:50:THR:HG23	2.17	0.45
1:B:507:ILE:HD13	1:B:534:GLU:HG3	1.99	0.45
1:C:481:SER:O	1:C:552:HIS:CE1	2.69	0.45
1:C:503:SER:HB2	1:C:532:ALA:HB2	1.99	0.44
1:B:503:SER:HB2	1:B:532:ALA:HB2	2.00	0.44
1:C:188:PHE:CZ	1:C:445:LYS:HE2	2.53	0.44
1:A:50:THR:HB	1:C:505:ILE:HD11	2.00	0.44
1:C:586:ASN:ND2	1:C:586:ASN:C	2.71	0.43
1:C:62:LEU:O	1:C:64:HIS:CE1	2.71	0.43
1:C:444:GLU:HG2	4:C:2460:HOH:O	2.19	0.43
1:A:91:ILE:HA	1:A:94:LEU:HD22	2.01	0.43
1:B:72:ASP:HA	1:B:73:PRO:HD2	1.89	0.43
1:C:208:PRO:HA	1:C:209:PRO:HD3	1.94	0.43
1:A:126:ASN:HB3	1:A:129:ALA:HB2	2.00	0.43
1:B:359:PRO:HG2	1:B:375:PHE:CE1	2.54	0.42
1:D:62:LEU:O	1:D:64:HIS:CE1	2.72	0.42
1:D:247:LYS:NZ	4:D:2333:HOH:O	2.50	0.42
1:A:586:ASN:C	1:A:586:ASN:HD22	2.22	0.42
1:D:417:VAL:HG12	1:D:428:ILE:HG12	2.02	0.42
1:A:240:GLN:O	1:A:244:VAL:HG22	2.19	0.42
1:A:141:GLN:HG2	1:A:397:TYR:CD1	2.55	0.42
1:C:129:ALA:HB3	1:C:396:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:O	1:A:64:HIS:CE1	2.73	0.41
1:D:459:ASP:HA	1:D:460:PRO:HD3	1.90	0.41
1:D:503:SER:HB2	1:D:532:ALA:HB2	2.02	0.41
1:A:158:ALA:HB1	1:A:199:PHE:CE1	2.56	0.41
1:B:418:ASN:OD1	1:B:418:ASN:C	2.58	0.41
1:D:46:ASP:O	1:D:49:ASN:HB3	2.21	0.41
1:B:482:TYR:HA	1:B:483:GLY:HA2	1.75	0.41
1:C:352:VAL:HA	1:C:353:PRO:HD3	1.95	0.40
1:B:360:PHE:CD1	1:B:369:GLN:HG2	2.55	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	A	595/598 (100%)	585 (98%)	10 (2%)	0	100	100
1	B	595/598 (100%)	584 (98%)	11 (2%)	0	100	100
1	C	595/598 (100%)	582 (98%)	11 (2%)	2 (0%)	41	46
1	D	595/598 (100%)	585 (98%)	9 (2%)	1 (0%)	47	55
All	All	2380/2392 (100%)	2336 (98%)	41 (2%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	336	LEU
1	D	372	PHE
1	C	48	ASP

### 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	490/491 (100%)	474 (97%)	16 (3%)	38	49
1	B	490/491 (100%)	471 (96%)	19 (4%)	32	41
1	C	490/491 (100%)	472 (96%)	18 (4%)	34	43
1	D	490/491 (100%)	469 (96%)	21 (4%)	29	36
All	All	1960/1964 (100%)	1886 (96%)	74 (4%)	33	42

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	85	SER
1	A	89	LYS
1	A	94	LEU
1	A	103	GLU
1	A	178	ASP
1	A	184	GLU
1	A	218	GLU
1	A	369	GLN
1	A	382	SER
1	A	395	VAL
1	A	424	LYS
1	A	478	PHE
1	A	488	VAL
1	A	507	ILE
1	A	586	ASN
1	B	5	ASP
1	B	48	ASP
1	B	50	THR
1	B	85	SER
1	B	103	GLU
1	B	181	LYS
1	B	184	GLU
1	B	271	GLU

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Mol	Chain	Res	Type
1	B	340	TYR
1	B	369	GLN
1	B	382	SER
1	B	426	GLU
1	B	447	GLU
1	B	478	PHE
1	B	481	SER
1	B	488	VAL
1	B	508	ASP
1	B	526	LYS
1	B	586	ASN
1	C	48	ASP
1	C	85	SER
1	C	94	LEU
1	C	179	SER
1	C	218	GLU
1	C	234	VAL
1	C	337	TYR
1	C	369	GLN
1	C	382	SER
1	C	395	VAL
1	C	424	LYS
1	C	437	GLU
1	C	444	GLU
1	C	452	LYS
1	C	478	PHE
1	C	481	SER
1	C	508	ASP
1	C	586	ASN
1	D	5	ASP
1	D	12	LYS
1	D	30	VAL
1	D	48	ASP
1	D	66	ASP
1	D	85	SER
1	D	89	LYS
1	D	171	GLU
1	D	178	ASP
1	D	218	GLU
1	D	337	TYR
1	D	340	TYR
1	D	363	GLU

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Mol	Chain	Res	Type
1	D	375	PHE
1	D	382	SER
1	D	395	VAL
1	D	428	ILE
1	D	478	PHE
1	D	481	SER
1	D	507	ILE
1	D	586	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	342	ASN
1	A	586	ASN
1	B	342	ASN
1	B	586	ASN
1	C	192	GLN
1	C	342	ASN
1	C	586	ASN
1	D	192	GLN
1	D	342	ASN
1	D	586	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z  > 2$
2	PO4	C	598	-	4,4,4	0.97	0	6,6,6	0.81	0
2	PO4	A	601	-	4,4,4	1.24	0	6,6,6	0.55	0
2	PO4	B	600	-	4,4,4	1.48	0	6,6,6	1.12	0
2	PO4	C	602	-	4,4,4	0.99	0	6,6,6	0.38	0
2	PO4	D	600	-	4,4,4	1.36	0	6,6,6	1.04	0
2	PO4	A	602	-	4,4,4	1.08	0	6,6,6	0.69	0
2	PO4	D	601	-	4,4,4	1.29	0	6,6,6	0.59	0
2	PO4	B	602	-	4,4,4	0.92	0	6,6,6	0.55	0
2	PO4	C	601	-	4,4,4	1.21	0	6,6,6	0.69	0
2	PO4	B	601	-	4,4,4	1.28	0	6,6,6	0.52	0
2	PO4	D	602	-	4,4,4	0.87	0	6,6,6	0.68	0
2	PO4	D	598	-	4,4,4	0.97	0	6,6,6	1.07	0
2	PO4	A	600	-	4,4,4	1.29	0	6,6,6	0.62	0
2	PO4	C	600	-	4,4,4	1.50	1 (25%)	6,6,6	0.62	0
2	PO4	B	598	-	4,4,4	0.94	0	6,6,6	0.85	0
2	PO4	A	598	-	4,4,4	1.05	0	6,6,6	0.76	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	PO4	P-O2	-2.07	1.48	1.54

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 ⓘ

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, 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	A	597/598 (99%)	-0.88	8 (1%) 77 75	18, 25, 46, 81	2 (0%)
1	B	597/598 (99%)	-0.93	3 (0%) 91 90	16, 23, 42, 76	2 (0%)
1	C	597/598 (99%)	-0.92	3 (0%) 91 90	17, 25, 43, 79	3 (0%)
1	D	597/598 (99%)	-0.90	7 (1%) 79 77	17, 25, 45, 69	1 (0%)
All	All	2388/2392 (99%)	-0.91	21 (0%) 84 83	16, 25, 44, 81	8 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	PRO	6.7
1	A	48	ASP	5.2
1	B	47	PRO	5.1
1	C	48	ASP	5.0
1	B	48	ASP	4.4
1	C	47	PRO	3.6
1	A	103	GLU	3.2
1	D	48	ASP	3.0
1	B	526	LYS	3.0
1	D	526	LYS	2.9
1	D	47	PRO	2.8
1	A	461	ASP	2.8
1	A	102	PRO	2.7
1	D	103	GLU	2.4
1	A	46	ASP	2.3
1	C	461	ASP	2.3
1	D	461	ASP	2.3
1	D	49	ASN	2.2
1	A	50	THR	2.1
1	D	102	PRO	2.1
1	A	526	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	D	602	5/5	0.94	0.12	21,24,36,36	5
2	PO4	A	601	5/5	0.95	0.23	17,23,29,31	5
2	PO4	B	601	5/5	0.96	0.21	22,22,25,25	5
2	PO4	B	602	5/5	0.96	0.10	16,22,27,29	5
2	PO4	A	600	5/5	0.96	0.16	20,25,31,35	5
2	PO4	D	601	5/5	0.97	0.33	14,14,22,22	5
2	PO4	B	600	5/5	0.97	0.09	17,19,21,28	5
2	PO4	C	601	5/5	0.97	0.22	25,27,32,35	5
2	PO4	C	602	5/5	0.97	0.09	16,18,23,23	5
2	PO4	D	600	5/5	0.97	0.14	17,17,23,25	5
2	PO4	A	602	5/5	0.97	0.09	11,18,32,33	5
3	CA	C	599	1/1	0.98	0.03	27,27,27,27	0
2	PO4	C	600	5/5	0.98	0.12	18,18,23,29	5
3	CA	B	599	1/1	0.99	0.03	26,26,26,26	0
2	PO4	D	598	5/5	0.99	0.05	26,26,29,29	0
2	PO4	C	598	5/5	0.99	0.05	26,29,30,32	0
3	CA	D	599	1/1	0.99	0.03	30,30,30,30	0
2	PO4	B	598	5/5	0.99	0.05	21,21,23,29	0
2	PO4	A	598	5/5	0.99	0.06	25,25,30,31	0
3	CA	A	599	1/1	1.00	0.02	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.