



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:28 am BST

PDB ID : 2R8Z
Title : Crystal structure of YrbI phosphatase from Escherichia coli in complex with a phosphate and a calcium ion
Authors : Tsodikov, O.V.; Aggarwal, P.; Rubin, J.R.; Stuckey, J.A.; Woodard, R.W.; Biswas, T.
Deposited on : 2007-09-11
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

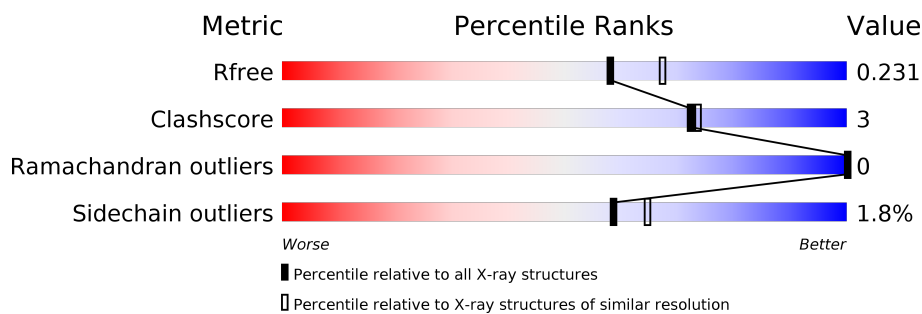
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	188	92% . .
1	B	188	91% 5% . .
1	C	188	91% . . .
1	D	188	86% 10% . .
1	E	188	84% 10% . 5%
1	F	188	86% 10% . .
1	G	188	87% 9% . .

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Mol	Chain	Length	Quality of chain
1	H	188	<div><div></div><div>88%</div><div>7%<div></div><div></div></div></div>
1	I	188	<div><div></div><div>89%</div><div>7%<div></div><div></div></div></div>
1	J	188	<div><div></div><div>85%</div><div>11%<div></div><div></div></div></div>
1	K	188	<div><div></div><div>92%</div><div><div></div><div></div></div></div>
1	L	188	<div><div></div><div>93%</div><div><div></div><div></div></div></div>
1	M	188	<div><div></div><div>91%</div><div>5%<div></div><div></div></div></div>
1	N	188	<div><div></div><div>89%</div><div>7%<div></div><div></div></div></div>
1	O	188	<div><div></div><div>90%</div><div><div></div><div></div>5%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24342 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.

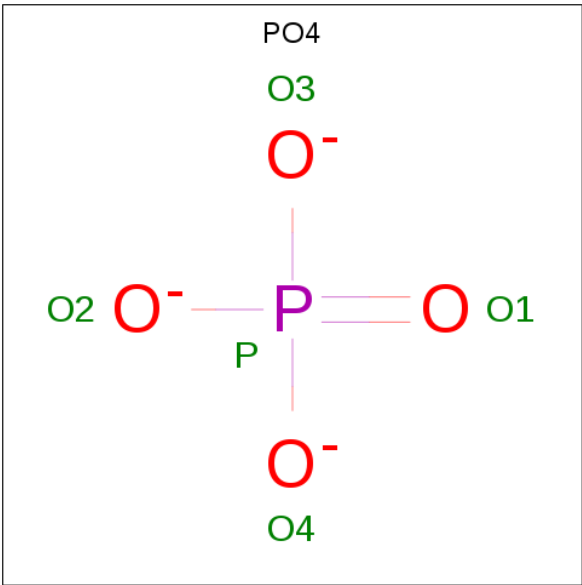
- Molecule 1 is a protein called 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	B	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	C	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	D	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	E	178	Total	C	N	O	S	0	0	0
			1332	842	228	255	7			
1	F	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	G	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	H	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	I	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	J	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	K	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	L	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	M	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	N	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	O	178	Total	C	N	O	S	0	0	0
			1332	842	228	255	7			
1	P	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Ca	0	0
			1	1		
2	G	1	Total	Ca	0	0
			1	1		
2	J	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	K	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	I	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	N	1	Total	Ca	0	0
			1	1		
2	O	1	Total	Ca	0	0
			1	1		
2	L	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		
2	M	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	211	Total	O	0	0
			211	211		
4	B	188	Total	O	0	0
			188	188		
4	C	210	Total	O	0	0
			210	210		
4	D	221	Total	O	0	0
			221	221		
4	E	227	Total	O	0	0
			227	227		
4	F	192	Total	O	0	0
			192	192		
4	G	190	Total	O	0	0
			190	190		
4	H	192	Total	O	0	0
			192	192		
4	I	110	Total	O	0	0
			110	110		
4	J	124	Total	O	0	0
			124	124		
4	K	105	Total	O	0	0
			105	105		
4	L	114	Total	O	0	0
			114	114		
4	M	118	Total	O	0	0
			118	118		
4	N	140	Total	O	0	0
			140	140		
4	O	122	Total	O	0	0
			122	122		
4	P	134	Total	O	0	0
			134	134		

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. 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. 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.

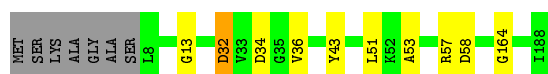
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain A: 



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain B: 




- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain C: 




- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain D: 




- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain E: 



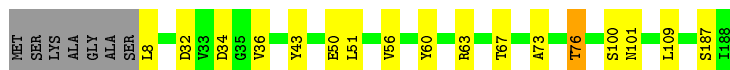
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain F: 



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain G: 87% 9% . .



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain H: 88% 7% . .



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain I: 89% 7% .



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain J: 85% 11% .



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain K: 92% . .



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain L: 93% . .



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain M: 91% 5% . .



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain N: 89% 7% . .



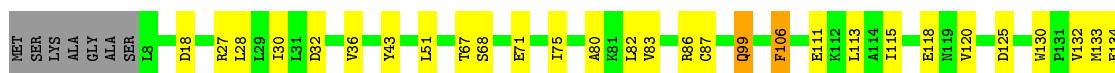
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain O: 90% . . 5%



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain P: 78% 18% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.37Å 156.91Å 114.05Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 38.43 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.10) 88.5 (38.43-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.231 0.185 , 0.231	Depositor DCC
R_{free} test set	9662 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24342	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: PO4, CA

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	0.38	0/1372	0.53	0/1858
1	B	0.36	0/1372	0.52	0/1858
1	C	0.38	0/1372	0.51	0/1858
1	D	0.39	0/1372	0.53	0/1858
1	E	0.39	0/1348	0.52	0/1827
1	F	0.38	0/1372	0.52	0/1858
1	G	0.38	0/1372	0.54	0/1858
1	H	0.38	0/1372	0.54	0/1858
1	I	0.33	0/1372	0.48	0/1858
1	J	0.33	0/1372	0.48	0/1858
1	K	0.32	0/1372	0.47	0/1858
1	L	0.32	0/1372	0.47	0/1858
1	M	0.33	0/1372	0.49	0/1858
1	N	0.34	0/1372	0.50	0/1858
1	O	0.34	0/1348	0.49	0/1827
1	P	0.86	5/1372 (0.4%)	0.73	4/1858 (0.2%)
All	All	0.41	5/21904 (0.0%)	0.52	4/29666 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	134	GLU	C-O	8.66	1.39	1.23
1	P	86	ARG	CZ-NH1	8.13	1.43	1.33
1	P	106	PHE	CG-CD1	5.92	1.47	1.38
1	P	136	VAL	C-O	-5.89	1.12	1.23
1	P	111	GLU	CD-OE1	5.62	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	106	PHE	CB-CG-CD2	-8.77	114.66	120.80
1	P	106	PHE	CG-CD2-CE2	-7.97	112.03	120.80
1	P	86	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	P	106	PHE	CD1-CG-CD2	6.11	126.25	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	1356	0	1385	5	0
1	B	1356	0	1385	7	0
1	C	1356	0	1385	6	0
1	D	1356	0	1385	14	0
1	E	1332	0	1361	17	0
1	F	1356	0	1385	14	0
1	G	1356	0	1385	13	0
1	H	1356	0	1385	10	0
1	I	1356	0	1385	7	0
1	J	1356	0	1385	12	0
1	K	1356	0	1385	6	0
1	L	1356	0	1385	4	0
1	M	1356	0	1385	6	0
1	N	1356	0	1385	9	0
1	O	1332	0	1361	4	0
1	P	1356	0	1385	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	1	0
3	H	5	0	0	1	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
4	A	211	0	0	7	0
4	B	188	0	0	1	0
4	C	210	0	0	2	0
4	D	221	0	0	3	0
4	E	227	0	0	6	0
4	F	192	0	0	3	0
4	G	190	0	0	4	0
4	H	192	0	0	4	0
4	I	110	0	0	1	0
4	J	124	0	0	0	0
4	K	105	0	0	1	0
4	L	114	0	0	0	0
4	M	118	0	0	0	0
4	N	140	0	0	2	0
4	O	122	0	0	0	0
4	P	134	0	0	11	0
All	All	24342	0	22112	147	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 3.

All (147) 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:87:CYS:SG	4:P:336:HOH:O	2.26	0.93
3:H:209:PO4:O2	4:H:212:HOH:O	1.91	0.88
1:E:105:ALA:HB2	4:E:379:HOH:O	1.73	0.87
1:P:82:LEU:HG	4:P:331:HOH:O	1.74	0.86
1:F:89:THR:HB	4:F:367:HOH:O	1.74	0.86
1:P:130:TRP:HZ3	4:P:346:HOH:O	1.61	0.82
1:E:99:GLN:HG2	4:E:214:HOH:O	1.78	0.82
1:P:27:ARG:HB2	1:P:115:ILE:CD1	2.10	0.81
1:P:27:ARG:HB2	1:P:115:ILE:HD11	1.64	0.79
3:D:205:PO4:O2	4:D:210:HOH:O	2.01	0.78
1:E:99:GLN:HB2	4:E:210:HOH:O	1.86	0.76
1:D:63:ARG:HE	1:D:186:GLN:HE22	1.31	0.75
3:A:202:PO4:O2	4:A:205:HOH:O	2.11	0.69
1:P:120:VAL:HG13	4:P:312:HOH:O	1.94	0.68
1:P:80:ALA:HB3	4:P:331:HOH:O	1.94	0.67
4:A:376:HOH:O	1:D:187:SER:HB3	1.96	0.66
1:E:99:GLN:HB3	4:E:356:HOH:O	1.95	0.66
1:G:67:THR:HG23	4:G:258:HOH:O	1.95	0.65
1:J:56:VAL:HG21	1:K:34:ASP:HB3	1.78	0.65
1:P:30:ILE:HG21	1:P:75:ILE:HD12	1.79	0.63
1:F:42:ILE:HD12	1:F:52:LYS:HZ3	1.64	0.63
1:G:76:THR:HG21	4:G:248:HOH:O	1.98	0.63
1:G:63:ARG:O	1:G:67:THR:HG22	1.99	0.62
1:E:99:GLN:CB	4:E:356:HOH:O	2.48	0.61
1:M:56:VAL:HG12	1:N:42:ILE:HG12	1.82	0.61
1:D:39:ASP:OD1	4:D:254:HOH:O	2.16	0.60
1:N:99:GLN:HG3	4:N:289:HOH:O	2.00	0.60
1:P:99:GLN:NE2	4:P:253:HOH:O	2.33	0.60
1:D:63:ARG:HE	1:D:186:GLN:NE2	2.00	0.60
1:P:133:MET:SD	4:P:335:HOH:O	2.56	0.59
1:I:89:THR:HG21	4:I:292:HOH:O	2.01	0.59
1:G:8:LEU:N	4:G:360:HOH:O	2.35	0.58
1:P:27:ARG:HB2	1:P:115:ILE:HD12	1.83	0.58
1:E:55:ASN:HD22	1:E:58:ASP:H	1.50	0.58
1:P:149:LEU:HD11	4:P:335:HOH:O	2.04	0.58
1:P:132:VAL:HB	4:P:338:HOH:O	2.05	0.56
1:E:110:LEU:HD22	1:E:115:ILE:HG23	1.88	0.56
1:F:28:LEU:HD21	1:F:109:LEU:HD13	1.86	0.56
1:I:43:TYR:HB2	1:I:51:LEU:HB2	1.88	0.56
1:D:63:ARG:O	1:D:67:THR:HB	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ARG:O	1:E:67:THR:HB	2.06	0.55
1:K:56:VAL:HG21	1:L:34:ASP:HB3	1.88	0.55
1:G:56:VAL:HG21	1:H:34:ASP:HB3	1.89	0.55
1:F:67:THR:HG23	4:F:345:HOH:O	2.07	0.54
1:E:68:SER:HB3	1:E:179:LYS:HD3	1.89	0.54
1:K:55:ASN:HD22	1:K:58:ASP:H	1.56	0.53
1:F:56:VAL:HG21	1:G:34:ASP:HB3	1.89	0.53
1:I:56:VAL:HG21	1:J:34:ASP:HB3	1.90	0.53
1:B:13:GLY:HA2	4:H:347:HOH:O	2.09	0.53
1:E:111:GLU:HG3	1:N:103:LEU:HD13	1.90	0.52
1:O:63:ARG:O	1:O:67:THR:HG22	2.10	0.52
1:C:67:THR:HG23	4:C:378:HOH:O	2.09	0.51
1:F:42:ILE:CD1	1:F:52:LYS:NZ	2.73	0.51
1:J:68:SER:HB3	1:J:179:LYS:HD3	1.91	0.51
1:I:34:ASP:HB3	1:L:56:VAL:HG21	1.93	0.51
1:M:43:TYR:HB2	1:M:51:LEU:HB2	1.91	0.51
1:N:110:LEU:HD22	1:N:115:ILE:HG23	1.91	0.51
1:N:94:HIS:HD2	4:N:258:HOH:O	1.94	0.50
1:E:101:ASN:C	1:E:101:ASN:HD22	2.14	0.50
1:G:73:ALA:CB	1:G:109:LEU:HD11	2.41	0.50
1:P:106:PHE:HE2	1:P:120:VAL:HG11	1.77	0.50
1:A:56:VAL:HG21	1:B:34:ASP:HB3	1.94	0.49
1:P:83:VAL:CG1	4:P:336:HOH:O	2.60	0.49
1:D:94:HIS:HD2	4:D:259:HOH:O	1.96	0.49
1:B:57:ARG:HD2	4:B:335:HOH:O	2.12	0.49
1:J:150:ILE:HG23	1:J:156:VAL:HG21	1.95	0.48
1:A:94:HIS:HD2	4:A:261:HOH:O	1.95	0.48
1:C:68:SER:HB3	1:C:179:LYS:HD3	1.96	0.48
1:J:32:ASP:OD2	1:J:102:LYS:NZ	2.46	0.48
1:F:42:ILE:CD1	1:F:52:LYS:HZ3	2.25	0.48
1:C:8:LEU:N	4:C:394:HOH:O	2.45	0.48
1:K:43:TYR:HB2	1:K:51:LEU:HB2	1.95	0.47
1:F:32:ASP:HB2	1:F:36:VAL:HG21	1.97	0.47
1:I:68:SER:HB3	1:I:179:LYS:HD3	1.97	0.47
1:A:43:TYR:HB2	1:A:51:LEU:HB2	1.96	0.47
1:J:133:MET:O	1:J:136:VAL:HG22	2.15	0.47
1:G:76:THR:HG23	3:G:208:PO4:O3	2.15	0.47
1:N:43:TYR:HB2	1:N:51:LEU:HB2	1.96	0.47
1:P:71:GLU:HG2	1:P:113:LEU:HD11	1.97	0.46
1:P:83:VAL:HG12	4:P:336:HOH:O	2.14	0.46
1:B:32:ASP:HB2	1:B:36:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:O	1:A:67:THR:HG22	2.15	0.46
1:I:52:LYS:HE2	1:I:82:LEU:HD11	1.98	0.46
1:J:43:TYR:HB2	1:J:51:LEU:HB2	1.98	0.46
1:H:163:ARG:HD3	4:H:350:HOH:O	2.15	0.46
1:P:28:LEU:HB3	1:P:115:ILE:HD13	1.98	0.45
1:C:55:ASN:HD22	1:C:58:ASP:H	1.65	0.45
1:D:27:ARG:HB2	1:D:115:ILE:HD12	1.98	0.45
1:E:74:ILE:HD12	1:E:87:CYS:SG	2.56	0.45
4:A:402:HOH:O	1:D:163:ARG:NH1	2.49	0.45
1:F:8:LEU:N	4:F:352:HOH:O	2.50	0.45
1:I:175:LEU:HB2	1:I:180:LEU:HD22	1.99	0.45
1:B:43:TYR:HB2	1:B:51:LEU:HB2	1.99	0.45
1:J:63:ARG:O	1:J:67:THR:HG22	2.16	0.45
1:G:60:TYR:HB2	1:G:187:SER:HA	1.99	0.44
1:P:43:TYR:HB2	1:P:51:LEU:HB2	1.99	0.44
1:E:101:ASN:ND2	4:E:327:HOH:O	2.49	0.44
1:M:52:LYS:HE2	1:M:82:LEU:HD11	1.99	0.44
1:H:68:SER:HB3	1:H:179:LYS:HD2	2.00	0.44
1:F:68:SER:HB3	1:F:179:LYS:HD3	1.99	0.44
1:E:43:TYR:HB2	1:E:51:LEU:HB2	2.00	0.44
1:D:32:ASP:OD1	1:D:102:LYS:NZ	2.51	0.43
1:H:55:ASN:HD22	1:H:58:ASP:H	1.65	0.43
1:G:50:GLU:O	1:H:45:GLY:HA2	2.19	0.43
1:D:101:ASN:HD22	1:D:101:ASN:C	2.22	0.43
1:F:27:ARG:HB2	1:F:115:ILE:HD12	2.00	0.43
1:L:43:TYR:HB2	1:L:51:LEU:HB2	2.00	0.43
1:E:42:ILE:HG12	1:H:56:VAL:HG12	2.01	0.43
1:D:74:ILE:HD12	1:D:87:CYS:SG	2.58	0.43
1:N:52:LYS:HE2	1:N:82:LEU:HD11	2.00	0.43
1:H:28:LEU:HB3	1:H:115:ILE:HD13	2.00	0.43
1:M:60:TYR:HB2	1:M:187:SER:HA	2.01	0.43
1:M:55:ASN:O	1:M:58:ASP:HB2	2.19	0.42
1:D:58:ASP:OD1	1:D:164:GLY:HA2	2.19	0.42
1:E:99:GLN:HG3	1:E:101:ASN:H	1.84	0.42
1:F:42:ILE:HD12	1:F:52:LYS:NZ	2.29	0.42
1:O:101:ASN:HD21	1:O:103:LEU:HD12	1.84	0.42
1:G:43:TYR:HB2	1:G:51:LEU:HB2	2.00	0.42
1:P:68:SER:HB3	1:P:179:LYS:HD3	2.01	0.42
1:A:94:HIS:HE1	4:A:285:HOH:O	2.02	0.42
1:O:43:TYR:HB2	1:O:51:LEU:HB2	2.02	0.42
1:K:8:LEU:N	4:K:286:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ASP:OD1	1:B:164:GLY:HA2	2.19	0.42
1:E:50:GLU:O	1:F:45:GLY:HA2	2.20	0.42
1:J:52:LYS:HE2	1:J:82:LEU:HD11	2.02	0.42
1:P:32:ASP:HB3	1:P:36:VAL:HG21	2.01	0.42
1:G:32:ASP:HB3	1:G:36:VAL:HG21	2.01	0.41
1:J:96:TYR:CE1	1:J:109:LEU:HG	2.55	0.41
1:J:56:VAL:HG22	1:K:40:GLY:O	2.21	0.41
1:P:118:GLU:O	1:P:137:GLY:HA3	2.19	0.41
1:D:43:TYR:HB2	1:D:51:LEU:HB2	2.01	0.41
1:H:94:HIS:HD2	4:H:233:HOH:O	2.02	0.41
1:J:28:LEU:HD21	1:J:109:LEU:HD13	2.03	0.41
1:N:27:ARG:HB2	1:N:115:ILE:HD12	2.03	0.41
1:C:30:ILE:HG21	1:C:75:ILE:HD12	2.02	0.41
1:H:101:ASN:HD22	1:H:101:ASN:C	2.24	0.41
1:N:42:ILE:HG22	1:N:44:MET:HG3	2.02	0.41
1:F:55:ASN:HD22	1:F:58:ASP:H	1.68	0.41
1:G:100:SER:HA	4:G:374:HOH:O	2.20	0.41
1:M:55:ASN:HD22	1:M:58:ASP:H	1.68	0.41
1:P:67:THR:HG21	1:P:184:LYS:O	2.20	0.41
1:P:28:LEU:HD22	1:P:113:LEU:HD12	2.02	0.40
1:H:150:ILE:HB	1:H:151:PRO:HD3	2.04	0.40
4:A:376:HOH:O	1:D:187:SER:CB	2.61	0.40
1:B:53:ALA:HA	1:C:42:ILE:O	2.22	0.40
4:A:391:HOH:O	1:O:182:GLU:HG3	2.21	0.40
1:L:142:VAL:HA	1:L:157:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

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	A	179/188 (95%)	176 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	179/188 (95%)	178 (99%)	1 (1%)	0	100	100
1	C	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	D	179/188 (95%)	178 (99%)	1 (1%)	0	100	100
1	E	176/188 (94%)	174 (99%)	2 (1%)	0	100	100
1	F	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	G	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	H	179/188 (95%)	178 (99%)	1 (1%)	0	100	100
1	I	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	J	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	K	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	L	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	M	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	N	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	O	176/188 (94%)	172 (98%)	4 (2%)	0	100	100
1	P	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
All	All	2858/3008 (95%)	2822 (99%)	36 (1%)	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	142/147 (97%)	140 (99%)	2 (1%)	67	73
1	B	142/147 (97%)	141 (99%)	1 (1%)	84	88
1	C	142/147 (97%)	141 (99%)	1 (1%)	84	88
1	D	142/147 (97%)	138 (97%)	4 (3%)	43	47
1	E	139/147 (95%)	135 (97%)	4 (3%)	42	46
1	F	142/147 (97%)	138 (97%)	4 (3%)	43	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	142/147 (97%)	140 (99%)	2 (1%)	67	73
1	H	142/147 (97%)	138 (97%)	4 (3%)	43	47
1	I	142/147 (97%)	139 (98%)	3 (2%)	53	59
1	J	142/147 (97%)	140 (99%)	2 (1%)	67	73
1	K	142/147 (97%)	142 (100%)	0	100	100
1	L	142/147 (97%)	141 (99%)	1 (1%)	84	88
1	M	142/147 (97%)	140 (99%)	2 (1%)	67	73
1	N	142/147 (97%)	139 (98%)	3 (2%)	53	59
1	O	139/147 (95%)	136 (98%)	3 (2%)	52	57
1	P	142/147 (97%)	138 (97%)	4 (3%)	43	47
All	All	2266/2352 (96%)	2226 (98%)	40 (2%)	59	65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	187	SER
1	B	32	ASP
1	C	67	THR
1	D	67	THR
1	D	100	SER
1	D	101	ASN
1	D	109	LEU
1	E	24	GLU
1	E	67	THR
1	E	100	SER
1	E	101	ASN
1	F	76	THR
1	F	78	ARG
1	F	109	LEU
1	F	187	SER
1	G	76	THR
1	G	101	ASN
1	H	56	VAL
1	H	67	THR
1	H	101	ASN
1	H	187	SER
1	I	25	ASN

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Mol	Chain	Res	Type
1	I	49	GLU
1	I	181	ASP
1	J	125	ASP
1	J	187	SER
1	L	76	THR
1	M	101	ASN
1	M	187	SER
1	N	99	GLN
1	N	101	ASN
1	N	187	SER
1	O	76	THR
1	O	125	ASP
1	O	182	GLU
1	P	18	ASP
1	P	99	GLN
1	P	125	ASP
1	P	187	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	47	ASN
1	A	55	ASN
1	A	94	HIS
1	A	101	ASN
1	B	25	ASN
1	B	55	ASN
1	B	94	HIS
1	C	25	ASN
1	C	55	ASN
1	C	101	ASN
1	C	119	ASN
1	D	55	ASN
1	D	94	HIS
1	D	101	ASN
1	D	186	GLN
1	E	25	ASN
1	E	55	ASN
1	E	94	HIS
1	E	101	ASN
1	E	119	ASN

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Mol	Chain	Res	Type
1	F	25	ASN
1	F	47	ASN
1	F	55	ASN
1	F	101	ASN
1	F	119	ASN
1	G	25	ASN
1	G	55	ASN
1	G	99	GLN
1	G	101	ASN
1	G	119	ASN
1	H	25	ASN
1	H	55	ASN
1	H	94	HIS
1	H	101	ASN
1	I	55	ASN
1	I	101	ASN
1	J	55	ASN
1	J	101	ASN
1	K	55	ASN
1	K	99	GLN
1	K	101	ASN
1	L	55	ASN
1	L	94	HIS
1	L	101	ASN
1	M	25	ASN
1	M	55	ASN
1	M	101	ASN
1	N	55	ASN
1	N	94	HIS
1	N	101	ASN
1	N	119	ASN
1	O	55	ASN
1	O	101	ASN
1	P	25	ASN
1	P	47	ASN
1	P	101	ASN
1	P	119	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 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	$\# Z > 2$
3	PO4	N	215	2	4,4,4	0.93	0	6,6,6	2.23	2 (33%)
3	PO4	I	210	2	4,4,4	0.89	0	6,6,6	1.34	1 (16%)
3	PO4	P	217	2	4,4,4	0.90	0	6,6,6	1.87	3 (50%)
3	PO4	C	204	2	4,4,4	0.88	0	6,6,6	1.14	1 (16%)
3	PO4	F	207	2	4,4,4	0.92	0	6,6,6	2.11	2 (33%)
3	PO4	H	209	2	4,4,4	0.98	0	6,6,6	1.49	2 (33%)
3	PO4	L	213	2	4,4,4	0.93	0	6,6,6	1.31	1 (16%)
3	PO4	M	214	2	4,4,4	0.89	0	6,6,6	1.13	0
3	PO4	B	203	2	4,4,4	0.96	0	6,6,6	1.57	2 (33%)
3	PO4	J	211	2	4,4,4	0.93	0	6,6,6	1.00	0
3	PO4	E	206	2	4,4,4	0.97	0	6,6,6	1.60	2 (33%)
3	PO4	K	212	2	4,4,4	0.95	0	6,6,6	0.86	0
3	PO4	O	216	2	4,4,4	0.91	0	6,6,6	1.02	0
3	PO4	D	205	2	4,4,4	1.07	0	6,6,6	1.96	3 (50%)
3	PO4	A	202	2	4,4,4	1.01	0	6,6,6	1.30	1 (16%)
3	PO4	G	208	2	4,4,4	0.95	0	6,6,6	1.55	2 (33%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	207	PO4	O2-P-O1	-4.05	96.06	110.89
3	N	215	PO4	O4-P-O1	-4.05	96.07	110.89
3	D	205	PO4	O4-P-O2	-2.93	98.58	107.97
3	I	210	PO4	O3-P-O2	2.71	116.66	107.97
3	H	209	PO4	O4-P-O2	-2.61	99.60	107.97
3	E	206	PO4	O4-P-O2	-2.58	99.70	107.97
3	F	207	PO4	O3-P-O1	2.48	119.97	110.89
3	B	203	PO4	O4-P-O3	-2.43	100.16	107.97
3	P	217	PO4	O3-P-O2	2.40	115.67	107.97
3	L	213	PO4	O3-P-O1	2.40	119.67	110.89
3	E	206	PO4	O3-P-O2	2.35	115.50	107.97
3	H	209	PO4	O3-P-O2	2.33	115.44	107.97
3	P	217	PO4	O4-P-O2	-2.22	100.85	107.97
3	D	205	PO4	O3-P-O2	2.21	115.05	107.97
3	G	208	PO4	O3-P-O2	-2.20	100.90	107.97
3	A	202	PO4	O3-P-O2	2.16	114.90	107.97
3	N	215	PO4	O4-P-O3	2.15	114.87	107.97
3	P	217	PO4	O3-P-O1	-2.11	103.19	110.89
3	B	203	PO4	O3-P-O1	2.10	118.57	110.89
3	D	205	PO4	O3-P-O1	2.08	118.49	110.89
3	C	204	PO4	O4-P-O2	-2.06	101.35	107.97
3	G	208	PO4	O3-P-O1	2.06	118.42	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	209	PO4	1	0
3	D	205	PO4	1	0
3	A	202	PO4	1	0
3	G	208	PO4	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.