Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 08:50 PM EDT

PDB ID	:	4OMB
Title	:	Phosphate binding protein
Authors	:	Neznansky, A.; Opatowsky, Y.
Deposited on	:	2014-01-27
Resolution	:	1.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	Percentile Ranks	Value
Rfree		0.218
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		4.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
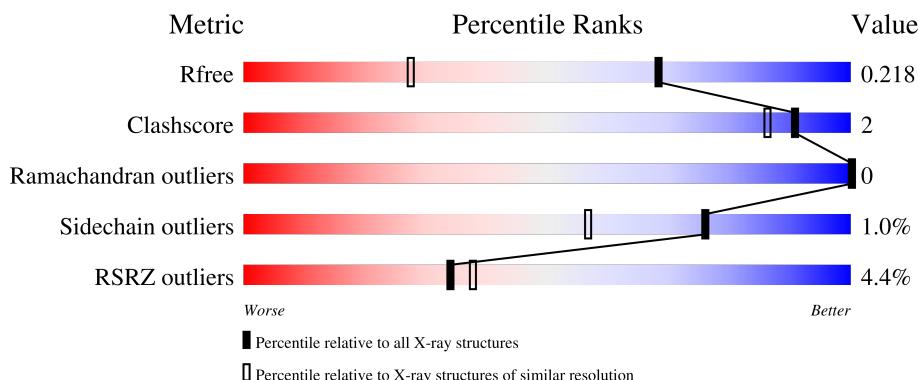
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	347	% 82% • 14%
1	B	347	3% 82% • 14%
1	C	347	% 80% 6% 14%
1	D	347	10% 82% • 14%
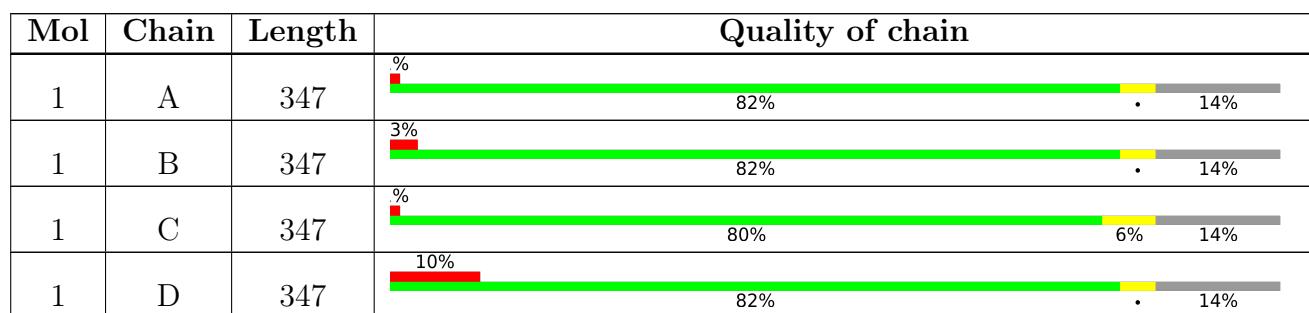
2 Entity composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9495 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 Phosphate binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2256	1437	378	434	7			
1	B	298	Total	C	N	O	S	0	0	0
			2256	1437	378	434	7			
1	C	298	Total	C	N	O	S	0	0	0
			2256	1437	378	434	7			
1	D	298	Total	C	N	O	S	0	0	0
			2256	1437	378	434	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q9Z9M3
A	-9	ASP	-	expression tag	UNP Q9Z9M3
A	-8	ILE	-	expression tag	UNP Q9Z9M3
A	-7	GLY	-	expression tag	UNP Q9Z9M3
A	-6	ILE	-	expression tag	UNP Q9Z9M3
A	-5	ASN	-	expression tag	UNP Q9Z9M3
A	-4	SER	-	expression tag	UNP Q9Z9M3
A	-3	ASP	-	expression tag	UNP Q9Z9M3
A	-2	PRO	-	expression tag	UNP Q9Z9M3
A	-1	ASN	-	expression tag	UNP Q9Z9M3
A	0	SER	-	expression tag	UNP Q9Z9M3
A	324	LYS	-	expression tag	UNP Q9Z9M3
A	325	LEU	-	expression tag	UNP Q9Z9M3
A	326	ALA	-	expression tag	UNP Q9Z9M3
A	327	ALA	-	expression tag	UNP Q9Z9M3
A	328	ALA	-	expression tag	UNP Q9Z9M3
A	329	LEU	-	expression tag	UNP Q9Z9M3
A	330	GLU	-	expression tag	UNP Q9Z9M3
A	331	HIS	-	expression tag	UNP Q9Z9M3
A	332	HIS	-	expression tag	UNP Q9Z9M3
A	333	HIS	-	expression tag	UNP Q9Z9M3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	334	HIS	-	expression tag	UNP Q9Z9M3
A	335	HIS	-	expression tag	UNP Q9Z9M3
A	336	HIS	-	expression tag	UNP Q9Z9M3
B	-10	MET	-	expression tag	UNP Q9Z9M3
B	-9	ASP	-	expression tag	UNP Q9Z9M3
B	-8	ILE	-	expression tag	UNP Q9Z9M3
B	-7	GLY	-	expression tag	UNP Q9Z9M3
B	-6	ILE	-	expression tag	UNP Q9Z9M3
B	-5	ASN	-	expression tag	UNP Q9Z9M3
B	-4	SER	-	expression tag	UNP Q9Z9M3
B	-3	ASP	-	expression tag	UNP Q9Z9M3
B	-2	PRO	-	expression tag	UNP Q9Z9M3
B	-1	ASN	-	expression tag	UNP Q9Z9M3
B	0	SER	-	expression tag	UNP Q9Z9M3
B	324	LYS	-	expression tag	UNP Q9Z9M3
B	325	LEU	-	expression tag	UNP Q9Z9M3
B	326	ALA	-	expression tag	UNP Q9Z9M3
B	327	ALA	-	expression tag	UNP Q9Z9M3
B	328	ALA	-	expression tag	UNP Q9Z9M3
B	329	LEU	-	expression tag	UNP Q9Z9M3
B	330	GLU	-	expression tag	UNP Q9Z9M3
B	331	HIS	-	expression tag	UNP Q9Z9M3
B	332	HIS	-	expression tag	UNP Q9Z9M3
B	333	HIS	-	expression tag	UNP Q9Z9M3
B	334	HIS	-	expression tag	UNP Q9Z9M3
B	335	HIS	-	expression tag	UNP Q9Z9M3
B	336	HIS	-	expression tag	UNP Q9Z9M3
C	-10	MET	-	expression tag	UNP Q9Z9M3
C	-9	ASP	-	expression tag	UNP Q9Z9M3
C	-8	ILE	-	expression tag	UNP Q9Z9M3
C	-7	GLY	-	expression tag	UNP Q9Z9M3
C	-6	ILE	-	expression tag	UNP Q9Z9M3
C	-5	ASN	-	expression tag	UNP Q9Z9M3
C	-4	SER	-	expression tag	UNP Q9Z9M3
C	-3	ASP	-	expression tag	UNP Q9Z9M3
C	-2	PRO	-	expression tag	UNP Q9Z9M3
C	-1	ASN	-	expression tag	UNP Q9Z9M3
C	0	SER	-	expression tag	UNP Q9Z9M3
C	324	LYS	-	expression tag	UNP Q9Z9M3
C	325	LEU	-	expression tag	UNP Q9Z9M3
C	326	ALA	-	expression tag	UNP Q9Z9M3
C	327	ALA	-	expression tag	UNP Q9Z9M3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	328	ALA	-	expression tag	UNP Q9Z9M3
C	329	LEU	-	expression tag	UNP Q9Z9M3
C	330	GLU	-	expression tag	UNP Q9Z9M3
C	331	HIS	-	expression tag	UNP Q9Z9M3
C	332	HIS	-	expression tag	UNP Q9Z9M3
C	333	HIS	-	expression tag	UNP Q9Z9M3
C	334	HIS	-	expression tag	UNP Q9Z9M3
C	335	HIS	-	expression tag	UNP Q9Z9M3
C	336	HIS	-	expression tag	UNP Q9Z9M3
D	-10	MET	-	expression tag	UNP Q9Z9M3
D	-9	ASP	-	expression tag	UNP Q9Z9M3
D	-8	ILE	-	expression tag	UNP Q9Z9M3
D	-7	GLY	-	expression tag	UNP Q9Z9M3
D	-6	ILE	-	expression tag	UNP Q9Z9M3
D	-5	ASN	-	expression tag	UNP Q9Z9M3
D	-4	SER	-	expression tag	UNP Q9Z9M3
D	-3	ASP	-	expression tag	UNP Q9Z9M3
D	-2	PRO	-	expression tag	UNP Q9Z9M3
D	-1	ASN	-	expression tag	UNP Q9Z9M3
D	0	SER	-	expression tag	UNP Q9Z9M3
D	324	LYS	-	expression tag	UNP Q9Z9M3
D	325	LEU	-	expression tag	UNP Q9Z9M3
D	326	ALA	-	expression tag	UNP Q9Z9M3
D	327	ALA	-	expression tag	UNP Q9Z9M3
D	328	ALA	-	expression tag	UNP Q9Z9M3
D	329	LEU	-	expression tag	UNP Q9Z9M3
D	330	GLU	-	expression tag	UNP Q9Z9M3
D	331	HIS	-	expression tag	UNP Q9Z9M3
D	332	HIS	-	expression tag	UNP Q9Z9M3
D	333	HIS	-	expression tag	UNP Q9Z9M3
D	334	HIS	-	expression tag	UNP Q9Z9M3
D	335	HIS	-	expression tag	UNP Q9Z9M3
D	336	HIS	-	expression tag	UNP Q9Z9M3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P ═ O O1

P

O⁻

O4
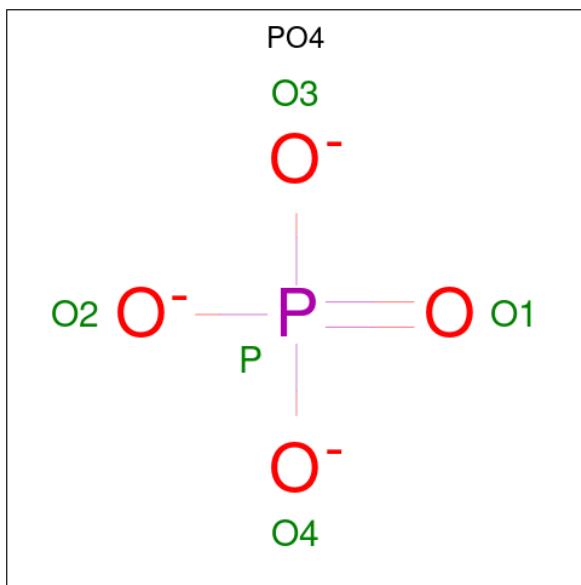
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0

- Molecule 3 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total 162	O 162	0	0

W O R L D W I D E
PDB
PROTEIN DATA BANK

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	122	Total 122	O 122	0	0
4	C	97	Total 97	O 97	0	0
4	D	66	Total 66	O 66	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphate binding protein
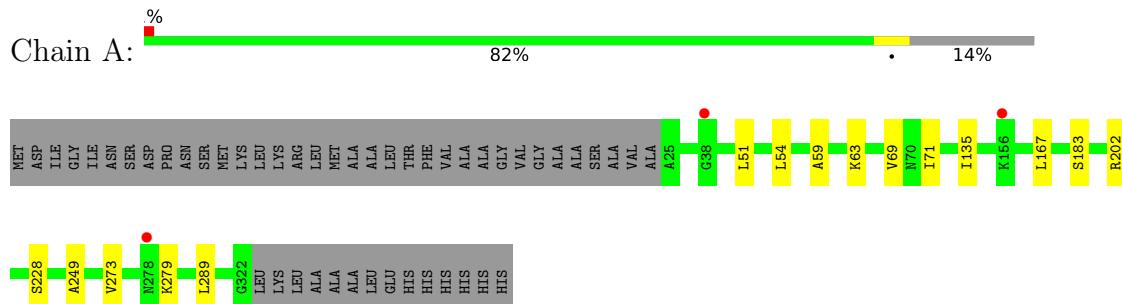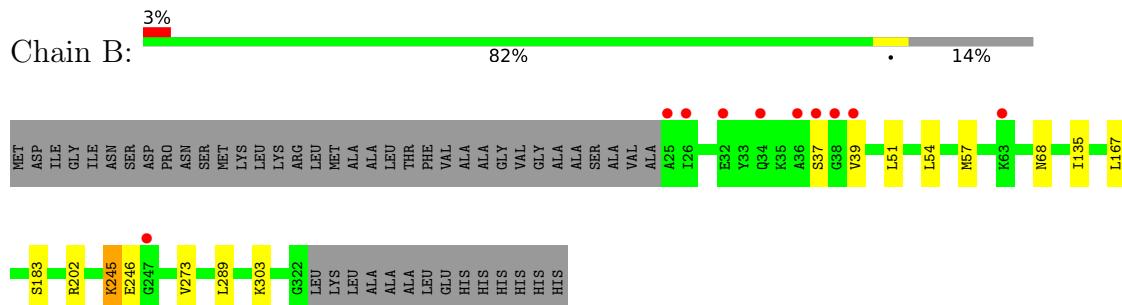


- Molecule 1: Phosphate binding protein

- Molecule 1: Phosphate binding protein

- Molecule 1: Phosphate binding protein

MET ASP ILE GLY ILE ASN SER ASP PRO ASN SER MET LYS LEU LYS ARG LEU MET ALA ALA LEU THR PHE VAL ALA ALA GLY VAL GLY ALA ALA SER ALA VAL ALA A25 S37 G38 V39 S40 G41 N42 L51 L54 Y62 K63 R64 L65 Y66 P67 N68 V69 N70 I71 T89

Q109 K110 Y111 G112 Y113 I135 D158 L167 D170 K173 S183 G231 K245 E246 G247 F250 V273 P277 N278 K279 P280 L281 D282 P283 L284 L289 T296 K312 K319 E320 L321 G322 LEU LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS

HIS HIS
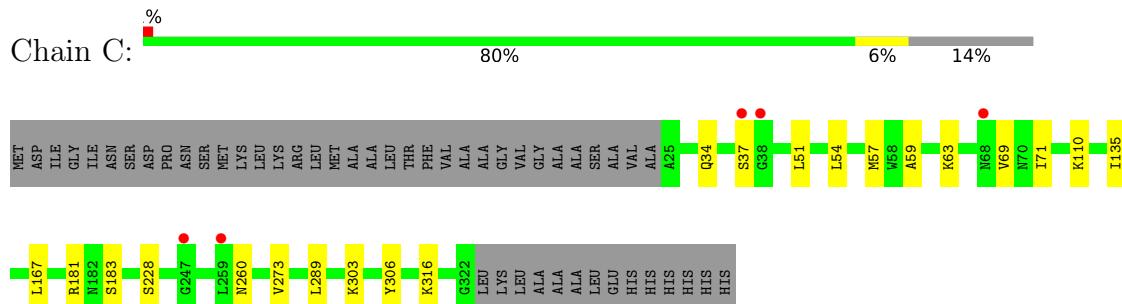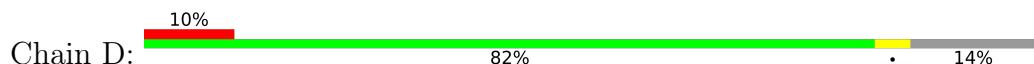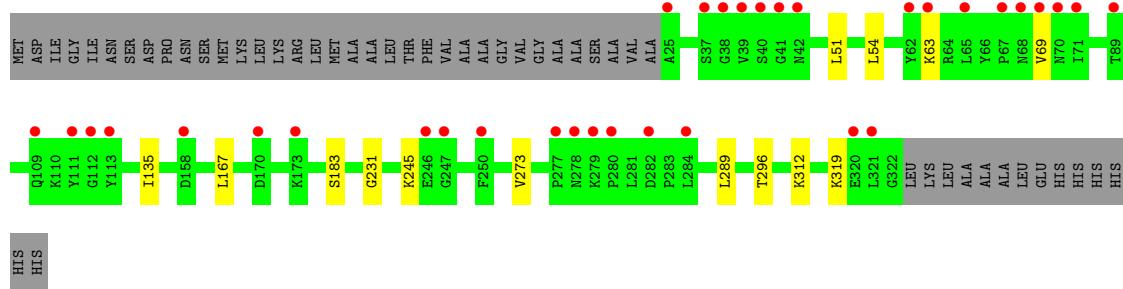
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	35.44Å 148.09Å 216.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.20 – 1.50 48.13 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (122.20-1.50) 98.3 (48.13-1.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.190 , 0.216 0.192 , 0.218	Depositor DCC
R_{free} test set	9127 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9495	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: PT, 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	0.78	1/2302 (0.0%)	0.79	1/3123 (0.0%)
1	B	0.71	1/2302 (0.0%)	0.76	1/3123 (0.0%)
1	C	0.75	2/2302 (0.1%)	0.77	1/3123 (0.0%)
1	D	0.66	2/2302 (0.1%)	0.72	0/3123
All	All	0.72	6/9208 (0.1%)	0.76	3/12492 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	183	SER	CB-OG	9.14	1.54	1.42
1	D	183	SER	CB-OG	7.68	1.52	1.42
1	B	183	SER	CB-OG	7.67	1.52	1.42
1	A	183	SER	CB-OG	6.86	1.51	1.42
1	C	183	SER	CA-CB	5.16	1.60	1.52
1	D	183	SER	CA-CB	5.09	1.60	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	202	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	181	ARG	NE-CZ-NH1	5.32	122.96	120.30

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	2256	0	2273	7	0
1	B	2256	0	2273	9	0
1	C	2256	0	2273	11	1
1	D	2256	0	2273	6	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	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	162	0	0	0	1
4	B	122	0	0	0	0
4	C	97	0	0	0	0
4	D	66	0	0	1	0
All	All	9495	0	9092	30	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (30) 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:B:245:LYS:HD2	1:B:246:GLU:H	1.39	0.87
1:C:135:ILE:HD12	1:C:167:LEU:HD11	1.78	0.66
1:C:51:LEU:HD23	1:C:54:LEU:HD12	1.78	0.65
1:D:51:LEU:HD23	1:D:54:LEU:HD12	1.79	0.64
1:B:51:LEU:HD23	1:B:54:LEU:HD12	1.82	0.60
1:A:51:LEU:HD23	1:A:54:LEU:HD12	1.83	0.60
1:A:249:ALA:HB1	1:C:110:LYS:HE3	1.84	0.58
1:A:273:VAL:HG11	1:A:289:LEU:HD11	1.86	0.58
1:B:245:LYS:HD2	1:B:246:GLU:N	2.14	0.58
1:A:249:ALA:CB	1:C:110:LYS:HE3	2.34	0.57
1:D:273:VAL:HG11	1:D:289:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG11	1:B:289:LEU:HD11	1.88	0.56
1:D:135:ILE:HD12	1:D:167:LEU:HD11	1.88	0.55
1:A:135:ILE:HD12	1:A:167:LEU:HD11	1.91	0.53
1:C:57:MET:SD	1:C:303:LYS:NZ	2.69	0.53
1:C:273:VAL:HG11	1:C:289:LEU:HD11	1.89	0.53
1:C:63:LYS:HD3	1:C:69:VAL:O	2.10	0.52
1:A:63:LYS:HD3	1:A:69:VAL:O	2.11	0.51
1:B:135:ILE:HD12	1:B:167:LEU:HD11	1.93	0.51
1:B:57:MET:SD	1:B:303:LYS:HE3	2.51	0.51
1:D:63:LYS:HD3	1:D:69:VAL:O	2.12	0.49
1:C:167:LEU:HD12	1:C:167:LEU:N	2.30	0.46
1:B:68:ASN:OD1	1:B:68:ASN:N	2.48	0.45
1:D:231:GLY:O	4:D:553:HOH:O	2.21	0.43
1:B:57:MET:CE	1:B:303:LYS:HE3	2.49	0.42
1:A:59:ALA:HB1	1:A:71:ILE:HD12	2.00	0.42
1:B:39:VAL:O	1:B:68:ASN:ND2	2.53	0.42
1:C:260:ASN:HD22	1:D:296:THR:HG23	1.85	0.41
1:C:135:ILE:HD12	1:C:167:LEU:CD1	2.49	0.41
1:C:59:ALA:HB1	1:C:71:ILE:HD12	2.03	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:TYR:O	1:D:312:LYS:NZ[1_655]	2.06	0.14
4:A:621:HOH:O	4:A:633:HOH:O[1_655]	2.14	0.06

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	296/347 (85%)	292 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	296/347 (85%)	291 (98%)	5 (2%)	0	100	100
1	C	296/347 (85%)	292 (99%)	4 (1%)	0	100	100
1	D	296/347 (85%)	292 (99%)	4 (1%)	0	100	100
All	All	1184/1388 (85%)	1167 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	241/276 (87%)	239 (99%)	2 (1%)	81	66
1	B	241/276 (87%)	239 (99%)	2 (1%)	81	66
1	C	241/276 (87%)	237 (98%)	4 (2%)	60	33
1	D	241/276 (87%)	239 (99%)	2 (1%)	81	66
All	All	964/1104 (87%)	954 (99%)	10 (1%)	76	57

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	SER
1	A	279	LYS
1	B	37	SER
1	B	245	LYS
1	C	34	GLN
1	C	37	SER
1	C	228	SER
1	C	316	LYS
1	D	245	LYS
1	D	319	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN
1	D	216	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	401	-	4,4,4	3.18	2 (50%)	6,6,6	1.31	1 (16%)
2	PO4	D	401	-	4,4,4	2.65	1 (25%)	6,6,6	1.18	1 (16%)
2	PO4	B	401	-	4,4,4	1.66	2 (50%)	6,6,6	0.88	0
2	PO4	A	401	-	4,4,4	1.72	1 (25%)	6,6,6	0.84	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PO4	P-O1	-5.06	1.38	1.50
2	D	401	PO4	P-O1	-4.88	1.39	1.50
2	C	401	PO4	P-O3	-3.75	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PO4	P-O2	-3.41	1.44	1.54
2	B	401	PO4	P-O1	-2.60	1.44	1.50
2	B	401	PO4	P-O2	-2.02	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	PO4	O3-P-O1	2.73	120.87	110.89
2	D	401	PO4	O2-P-O1	2.04	118.36	110.89

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, 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(Å²)	Q<0.9
1	A	298/347 (85%)	-0.34	3 (1%)	82	85	13, 21, 50, 81	0
1	B	298/347 (85%)	-0.19	10 (3%)	45	49	15, 26, 67, 87	0
1	C	298/347 (85%)	-0.22	5 (1%)	70	75	15, 27, 60, 75	0
1	D	298/347 (85%)	0.29	34 (11%)	5	4	17, 34, 74, 91	0
All	All	1192/1388 (85%)	-0.11	52 (4%)	34	38	13, 27, 63, 91	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	SER	5.0
1	D	278	ASN	4.6
1	D	69	VAL	4.5
1	D	68	ASN	4.4
1	D	38	GLY	4.0
1	B	247	GLY	3.7
1	B	37	SER	3.6
1	C	247	GLY	3.5
1	D	247	GLY	3.5
1	D	62	TYR	3.4
1	C	38	GLY	3.3
1	B	39	VAL	3.3
1	D	277	PRO	3.2
1	D	280	PRO	3.2
1	D	284	LEU	3.2
1	D	37	SER	3.1
1	B	38	GLY	3.1
1	D	279	LYS	2.9
1	D	63	LYS	2.8
1	C	68	ASN	2.7
1	D	70	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	111	TYR	2.7
1	D	42	ASN	2.7
1	B	34	GLN	2.6
1	A	38	GLY	2.6
1	D	41	GLY	2.6
1	D	89	THR	2.6
1	B	36	ALA	2.6
1	D	113	TYR	2.5
1	A	156	LYS	2.5
1	D	109	GLN	2.5
1	D	173	LYS	2.5
1	D	65	LEU	2.4
1	D	67	PRO	2.3
1	D	40	SER	2.3
1	D	321	LEU	2.3
1	D	112	GLY	2.3
1	A	278	ASN	2.3
1	D	246	GLU	2.2
1	B	25	ALA	2.2
1	D	282	ASP	2.2
1	D	71	ILE	2.2
1	D	170	ASP	2.1
1	D	25	ALA	2.1
1	B	26	ILE	2.1
1	B	63	LYS	2.1
1	D	158	ASP	2.1
1	B	32	GLU	2.1
1	D	250	PHE	2.1
1	C	259	LEU	2.1
1	D	320	GLU	2.0
1	D	39	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PT	B	402	1/1	0.67	0.06	118,118,118,118	0
3	PT	D	402	1/1	0.72	0.05	121,121,121,121	0
3	PT	C	402	1/1	0.78	0.06	110,110,110,110	0
3	PT	A	402	1/1	0.88	0.05	84,84,84,84	0
2	PO4	A	401	5/5	0.99	0.08	15,15,15,16	0
2	PO4	B	401	5/5	0.99	0.09	17,17,17,18	0
2	PO4	C	401	5/5	0.99	0.07	15,17,18,19	0
2	PO4	D	401	5/5	0.99	0.08	18,19,21,23	0

6.5 Other polymers (i)

There are no such residues in this entry.