



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:22 AM UTC

PDB ID : 2QY1 / pdb_00002qy1
Title : pectate lyase A31G/R236F from Xanthomonas campestris
Authors : Garron, M.L.; Shaya, D.
Deposited on : 2007-08-13
Resolution : 1.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

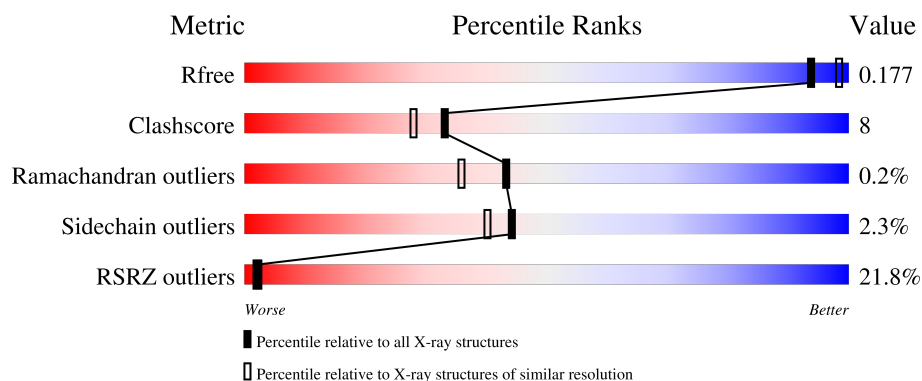
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	330	30% 85% 13%
1	B	330	13% 86% 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5654 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.

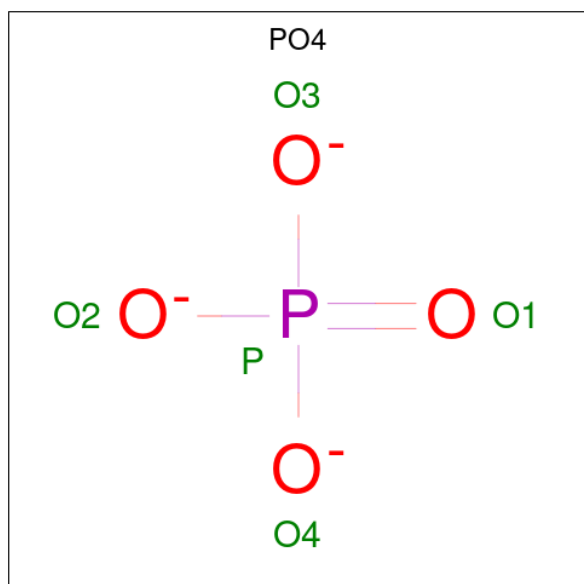
- Molecule 1 is a protein called Pectate lyase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	1	0
			2494	1564	430	494	6			
1	B	330	Total	C	N	O	S	0	1	0
			2494	1564	430	494	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	ALA	engineered mutation	UNP Q8P6Z9
A	236	PHE	ARG	engineered mutation	UNP Q8P6Z9
B	31	GLY	ALA	engineered mutation	UNP Q8P6Z9
B	236	PHE	ARG	engineered mutation	UNP Q8P6Z9

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

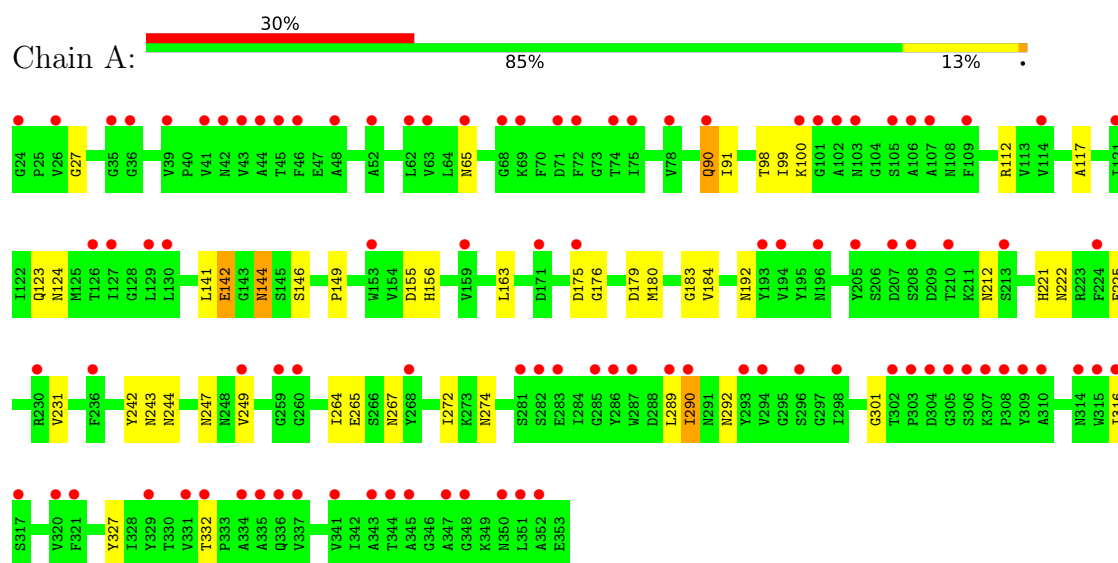
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	304	Total	O	0	0
			304	304		
3	B	352	Total	O	0	0
			352	352		

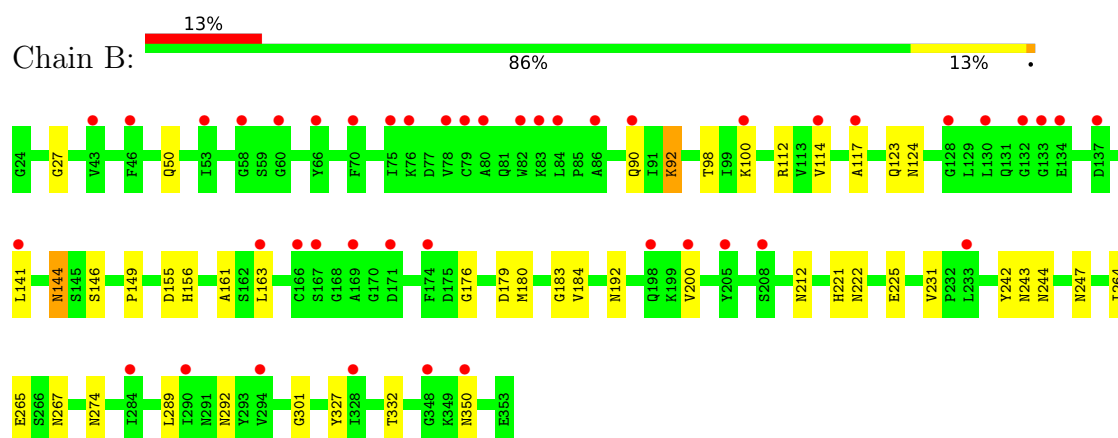
3 Residue-property plots

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: Pectate lyase II



• Molecule 1: Pectate lyase II



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.58Å 53.31Å 73.21Å 71.64° 80.15° 68.96°	Depositor
Resolution (Å)	21.20 – 1.90 21.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.1 (21.20-1.90) 86.1 (21.20-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.88 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.162 , 0.189 0.172 , 0.177	Depositor DCC
R_{free} test set	2392 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5654	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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

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	0.44	0/2548	0.72	0/3459
1	B	0.43	0/2548	0.70	1/3459 (0.0%)
All	All	0.44	0/5096	0.71	1/6918 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	VAL	N-CA-C	5.11	115.22	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2494	0	2403	40	0
1	B	2494	0	2403	36	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	304	0	0	2	0
3	B	352	0	0	1	0
All	All	5654	0	4806	76	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 8.

All (76) 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:A:98:THR:HG21	1:A:100:LYS:HE3	1.27	1.11
1:B:98:THR:HG21	1:B:100:LYS:HE3	1.36	1.03
1:A:98:THR:CG2	1:A:100:LYS:HE3	1.94	0.97
1:B:50:GLN:HE22	1:B:90:GLN:H	1.15	0.89
1:A:98:THR:HG22	1:A:100:LYS:HG3	1.55	0.87
1:A:175:ASP:CG	1:A:176:GLY:H	1.84	0.86
1:B:274:ASN:HD21	1:B:301:GLY:H	1.19	0.85
1:B:243:ASN:HD21	1:B:332:THR:H	1.21	0.83
1:B:98:THR:CG2	1:B:100:LYS:HE3	2.09	0.82
1:A:98:THR:CG2	1:A:100:LYS:HG3	2.09	0.82
1:A:274:ASN:HD21	1:A:301:GLY:H	1.24	0.82
1:B:98:THR:HG22	1:B:100:LYS:HG3	1.60	0.81
1:A:98:THR:HG21	1:A:100:LYS:CE	2.10	0.78
1:A:243:ASN:HD21	1:A:332:THR:H	1.32	0.77
1:B:98:THR:CG2	1:B:100:LYS:HG3	2.16	0.76
1:B:243:ASN:ND2	1:B:332:THR:H	1.90	0.69
1:B:92:LYS:HD3	1:B:114:VAL:HG13	1.76	0.67
1:A:192:ASN:H	1:A:222:ASN:HD22	1.43	0.66
1:B:192:ASN:H	1:B:222:ASN:HD22	1.44	0.66
1:A:243:ASN:ND2	1:A:332:THR:H	1.97	0.64
1:B:244:ASN:H	1:B:267:ASN:HD22	1.47	0.62
1:A:244:ASN:H	1:A:267:ASN:HD22	1.50	0.58
1:B:243:ASN:HD21	1:B:332:THR:N	1.97	0.58
1:B:98:THR:HG21	1:B:100:LYS:CE	2.23	0.58
1:A:90:GLN:NE2	3:A:502:HOH:O	2.36	0.58
1:A:144:ASN:C	1:A:144:ASN:HD22	2.12	0.57
1:B:183:GLY:H	1:B:212:ASN:HD22	1.50	0.57
1:A:192:ASN:H	1:A:222:ASN:ND2	2.03	0.56
1:B:92:LYS:HD2	3:B:457:HOH:O	2.06	0.55
1:B:149:PRO:HD2	1:B:184:VAL:HG22	1.89	0.55
1:A:183:GLY:H	1:A:212:ASN:HD22	1.55	0.55
1:B:144:ASN:HD22	1:B:144:ASN:C	2.14	0.55
1:B:192:ASN:H	1:B:222:ASN:ND2	2.05	0.55
1:A:267:ASN:H	1:A:292:ASN:HD22	1.56	0.53
1:A:175:ASP:CG	1:A:176:GLY:N	2.54	0.52
1:B:264:ILE:HB	1:B:289:LEU:HD23	1.93	0.50
1:B:274:ASN:ND2	1:B:301:GLY:H	2.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:ND2	1:A:146:SER:H	2.12	0.48
1:A:98:THR:CG2	1:A:100:LYS:CG	2.89	0.48
1:B:117:ALA:O	1:B:149:PRO:HA	2.14	0.48
1:A:65:ASN:ND2	3:A:645:HOH:O	2.47	0.48
1:B:123:GLN:HA	1:B:155:ASP:O	2.14	0.47
1:A:244:ASN:H	1:A:267:ASN:ND2	2.11	0.47
1:A:112:ARG:HE	1:A:142:GLU:CD	2.23	0.47
1:B:144:ASN:ND2	1:B:146:SER:H	2.13	0.47
1:A:149:PRO:HD2	1:A:184:VAL:HG22	1.96	0.46
1:B:27:GLY:HA2	1:B:327:TYR:CE2	2.51	0.46
1:A:91:ILE:HD11	1:A:99:ILE:HD11	1.98	0.46
1:B:225:GLU:HA	1:B:247:ASN:O	2.16	0.46
1:A:141:LEU:O	1:A:180:MET:HA	2.16	0.46
1:B:100:LYS:HE2	1:B:123:GLN:NE2	2.31	0.46
1:B:244:ASN:H	1:B:267:ASN:ND2	2.11	0.46
1:B:176:GLY:HA3	1:B:179:ASP:OD2	2.16	0.45
1:A:117:ALA:O	1:A:149:PRO:HA	2.16	0.45
1:A:225:GLU:HA	1:A:247:ASN:O	2.16	0.45
1:A:264:ILE:HB	1:A:289:LEU:HD23	1.99	0.45
1:A:267:ASN:H	1:A:292:ASN:ND2	2.16	0.44
1:B:141:LEU:O	1:B:180:MET:HA	2.18	0.44
1:A:98:THR:CG2	1:A:100:LYS:CE	2.78	0.44
1:B:242:TYR:HA	1:B:265:GLU:O	2.18	0.44
1:A:98:THR:HG23	1:A:100:LYS:HE3	1.93	0.43
1:A:176:GLY:HA3	1:A:179:ASP:OD2	2.17	0.43
1:B:267:ASN:H	1:B:292:ASN:HD22	1.66	0.43
1:A:124:ASN:HA	1:A:156:HIS:O	2.19	0.43
1:A:242:TYR:HA	1:A:265:GLU:O	2.19	0.43
1:A:221:HIS:CE1	1:A:243:ASN:HD22	2.36	0.42
1:B:124:ASN:HA	1:B:156:HIS:O	2.18	0.42
1:A:243:ASN:HD21	1:A:332:THR:N	2.09	0.42
1:B:90:GLN:HE21	1:B:112:ARG:HD2	1.84	0.42
1:B:221:HIS:HA	1:B:243:ASN:O	2.20	0.42
1:B:267:ASN:H	1:B:292:ASN:ND2	2.18	0.41
1:A:123:GLN:HA	1:A:155:ASP:O	2.19	0.41
1:B:221:HIS:CE1	1:B:243:ASN:HD22	2.39	0.41
1:A:27:GLY:HA2	1:A:327:TYR:CE2	2.56	0.41
1:A:289:LEU:C	1:A:290:ILE:HG13	2.47	0.40
1:A:249:VAL:HB	1:A:272:ILE:HG13	2.03	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	329/330 (100%)	316 (96%)	13 (4%)	0	100	100
1	B	329/330 (100%)	315 (96%)	13 (4%)	1 (0%)	36	29
All	All	658/660 (100%)	631 (96%)	26 (4%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	ALA

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	265/264 (100%)	258 (97%)	7 (3%)	40	35
1	B	265/264 (100%)	260 (98%)	5 (2%)	50	47
All	All	530/528 (100%)	518 (98%)	12 (2%)	44	40

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	142	GLU
1	A	144	ASN
1	A	163	LEU
1	A	231	VAL

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Mol	Chain	Res	Type
1	A	290	ILE
1	A	316	ILE
1	B	92	LYS
1	B	144	ASN
1	B	163	LEU
1	B	231	VAL
1	B	350	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	131	GLN
1	A	144	ASN
1	A	212	ASN
1	A	222	ASN
1	A	243	ASN
1	A	247	ASN
1	A	267	ASN
1	A	274	ASN
1	A	292	ASN
1	B	50	GLN
1	B	81	GLN
1	B	108	ASN
1	B	144	ASN
1	B	212	ASN
1	B	222	ASN
1	B	243	ASN
1	B	247	ASN
1	B	267	ASN
1	B	274	ASN
1	B	292	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	B	1	-	4,4,4	0.93	0	6,6,6	0.36	0
2	PO4	A	2	-	4,4,4	0.87	0	6,6,6	0.44	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/330 (100%)	1.59	100 (30%) ⓘ ⓘ	12, 21, 26, 33	1 (0%)
1	B	330/330 (100%)	1.26	44 (13%) ⓘ ⓘ	12, 21, 25, 27	1 (0%)
All	All	660/660 (100%)	1.43	144 (21%) ⓘ ⓘ	12, 21, 25, 33	2 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	ASP	5.1
1	A	171	ASP	5.0
1	B	100	LYS	4.7
1	A	306	SER	4.7
1	B	328	ILE	4.6
1	A	100	LYS	4.6
1	A	348	GLY	4.2
1	A	304	ASP	4.0
1	A	341	VAL	3.7
1	B	84	LEU	3.7
1	A	101	GLY	3.7
1	A	102	ALA	3.6
1	A	347	ALA	3.6
1	A	39	VAL	3.6
1	B	82	TRP	3.5
1	B	169	ALA	3.4
1	B	86	ALA	3.3
1	A	337	VAL	3.3
1	B	43	VAL	3.2
1	A	281	SER	3.2
1	A	205	TYR	3.2
1	A	303	PRO	3.2
1	A	331	VAL	3.2
1	A	106	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	60	GLY	3.1
1	B	78	VAL	3.1
1	A	48	ALA	3.1
1	A	78	VAL	3.0
1	A	315	TRP	3.0
1	A	351	LEU	3.0
1	B	114	VAL	3.0
1	B	290	ILE	3.0
1	A	334	ALA	2.9
1	A	352	ALA	2.9
1	A	41	VAL	2.9
1	A	309	TYR	2.9
1	A	44	ALA	2.8
1	B	132	GLY	2.8
1	B	198	GLN	2.8
1	B	134	GLU	2.8
1	B	167	SER	2.8
1	A	63	VAL	2.8
1	A	287	TRP	2.8
1	A	317	SER	2.7
1	A	45	THR	2.7
1	A	43	VAL	2.7
1	B	205	TYR	2.7
1	A	344	THR	2.7
1	A	320	VAL	2.7
1	A	308	PRO	2.7
1	A	207	ASP	2.6
1	A	282	SER	2.6
1	B	137[A]	ASP	2.6
1	B	90	GLN	2.6
1	A	42	ASN	2.6
1	B	79	CYS	2.6
1	A	75	ILE	2.6
1	B	80	ALA	2.6
1	A	153	TRP	2.5
1	A	307	LYS	2.5
1	A	316	ILE	2.5
1	A	268	TYR	2.5
1	A	46	PHE	2.5
1	A	90	GLN	2.5
1	A	305	GLY	2.4
1	A	105	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	260	GLY	2.4
1	B	128	GLY	2.4
1	B	70	PHE	2.4
1	A	350	ASN	2.4
1	B	348	GLY	2.4
1	A	208	SER	2.4
1	B	46	PHE	2.4
1	A	310	ALA	2.4
1	A	345	ALA	2.4
1	A	286	TYR	2.3
1	A	121	ILE	2.3
1	A	290	ILE	2.3
1	B	284	ILE	2.3
1	B	58	GLY	2.3
1	B	208	SER	2.3
1	A	126	THR	2.3
1	A	109	PHE	2.3
1	A	298	ILE	2.3
1	B	166	CYS	2.3
1	A	130	LEU	2.3
1	A	35	GLY	2.3
1	A	36	GLY	2.3
1	B	75	ILE	2.3
1	A	62	LEU	2.3
1	A	236	PHE	2.2
1	A	259	GLY	2.2
1	A	335	ALA	2.2
1	B	174	PHE	2.2
1	A	175	ASP	2.2
1	A	343	ALA	2.2
1	A	72	PHE	2.2
1	A	329	TYR	2.2
1	B	83	LYS	2.2
1	A	24	GLY	2.2
1	A	285	GLY	2.2
1	A	127	ILE	2.2
1	B	53	ILE	2.2
1	A	26	VAL	2.2
1	A	71	ASP	2.2
1	A	289	LEU	2.2
1	B	133	GLY	2.2
1	B	117	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	293	TYR	2.1
1	A	74	THR	2.1
1	A	194	VAL	2.1
1	A	65	ASN	2.1
1	A	296	SER	2.1
1	A	159	VAL	2.1
1	A	249	VAL	2.1
1	A	196	ASN	2.1
1	B	130	LEU	2.1
1	B	141	LEU	2.1
1	A	107	ALA	2.1
1	A	336	GLN	2.1
1	A	213	SER	2.1
1	A	210	THR	2.1
1	A	302	THR	2.1
1	A	68	GLY	2.1
1	A	103	ASN	2.1
1	A	114	VAL	2.1
1	B	294	VAL	2.1
1	B	163	LEU	2.1
1	A	52	ALA	2.1
1	A	193	TYR	2.0
1	B	66	TYR	2.0
1	B	350	ASN	2.0
1	A	294	VAL	2.0
1	A	129	LEU	2.0
1	B	233	LEU	2.0
1	A	230	ARG	2.0
1	A	283	GLU	2.0
1	A	69	LYS	2.0
1	B	76	LYS	2.0
1	A	224	PHE	2.0
1	A	321	PHE	2.0
1	A	332	THR	2.0
1	A	314	ASN	2.0
1	B	200	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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	A	2	5/5	0.89	0.23	33,33,34,34	0
2	PO4	B	1	5/5	0.94	0.16	23,24,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.