Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 08:57 PM EDT

PDB ID	:	5TOS
Title	:	Botrytis-induced kinase 1 (BIK1) from Arabidopsis thaliana
Authors	:	Hurlburt, N.K.; Lal, N.K.; Fisher, A.J.
Deposited on	:	2016-10-18
Resolution	:	2.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

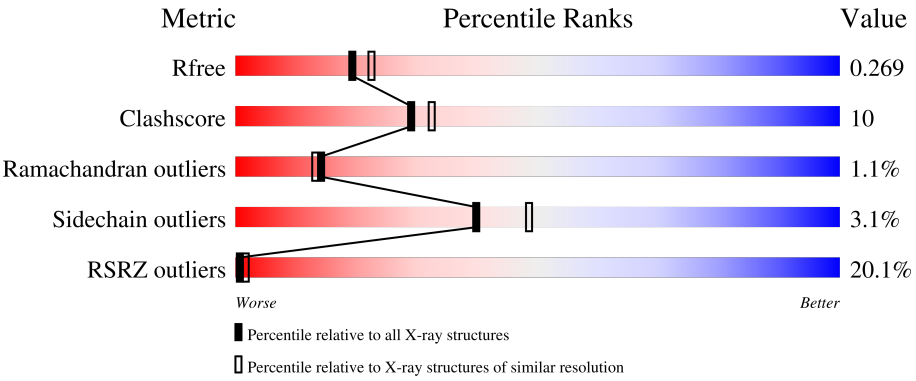
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	395	14% 57% 11% · 29%
1	B	395	15% 57% 13% · 29%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4671 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 Serine/threonine-protein kinase BIK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	P	S	0	0	0
			2257	1449	392	408	1	7			
1	B	280	Total	C	N	O	P	S	0	0	0
			2257	1449	392	408	1	7			

- Molecule 2 is water.

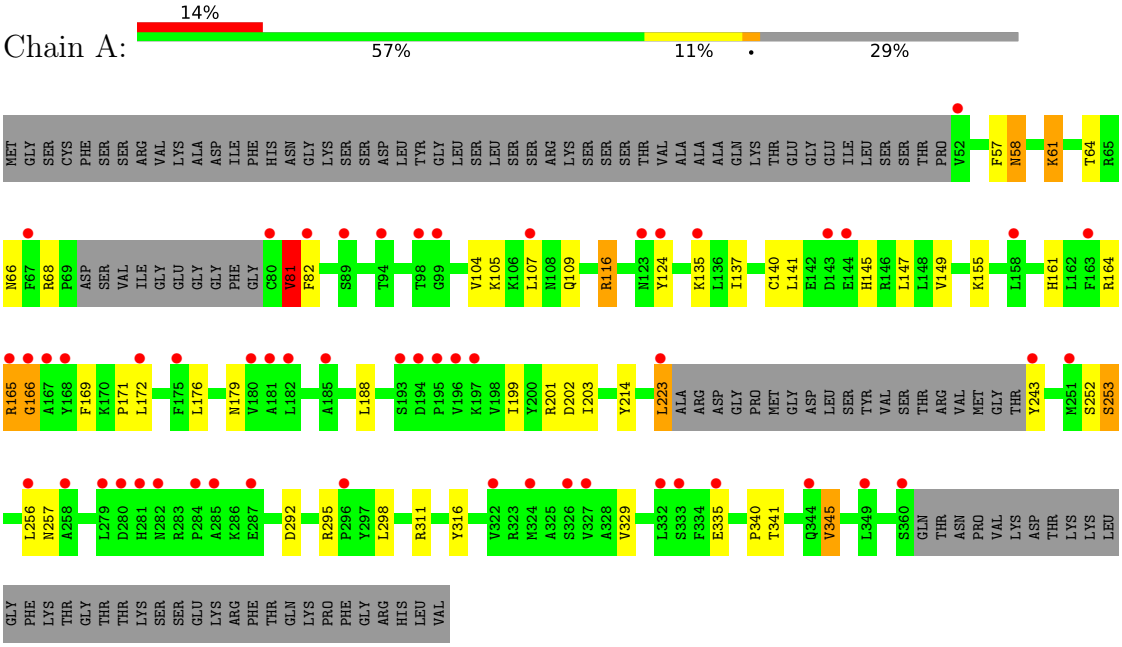
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	77	Total	O	0	0
			77	77		

3 Residue-property plots (i)

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.

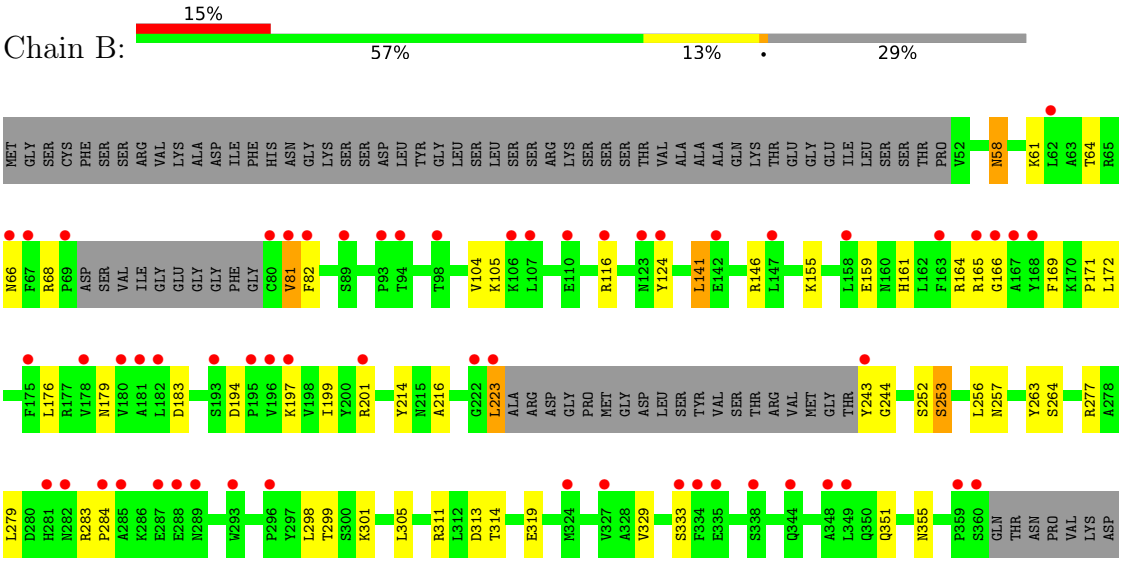
• Molecule 1: Serine/threonine-protein kinase BIK1

Chain A:



• Molecule 1: Serine/threonine-protein kinase BIK1

Chain B:



THR
LYS
LYS
LEU
GLY
PHE
LYS
THR
GLY
THR
THR
LYS
SER
SER
GLU
LYS
ARG
PHE
THR
GLN
LYS
PRO
PHE
GLY
ARG
HIS
LEU
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.19Å 72.09Å 93.88Å 90.00° 108.41° 90.00°	Depositor
Resolution (Å)	33.54 – 2.35 39.20 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.6 (33.54-2.35) 96.7 (39.20-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.238 , 0.268 0.243 , 0.269	Depositor DCC
R_{free} test set	1448 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4671	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3552e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SEP

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	0.25	0/2297	0.43	0/3106
1	B	0.25	0/2297	0.44	0/3106
All	All	0.25	0/4594	0.43	0/6212

There are no bond length outliers.

There are no bond angle outliers.

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	2257	0	2268	42	0
1	B	2257	0	2268	46	0
2	A	80	0	0	18	0
2	B	77	0	0	21	0
All	All	4671	0	4536	87	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 10.

All (87) 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:340:PRO:HG2	2:A:418:HOH:O	1.37	1.25
1:B:244:GLY:HA3	2:B:454:HOH:O	1.37	1.24
1:A:203:ILE:HG13	2:A:424:HOH:O	1.35	1.18
1:B:263:TYR:CD1	2:B:414:HOH:O	2.14	1.01
1:B:277:ARG:HD2	2:B:433:HOH:O	1.62	0.98
1:B:81:VAL:CG2	2:B:420:HOH:O	2.09	0.96
1:A:243:TYR:HB2	2:A:411:HOH:O	1.64	0.96
1:B:244:GLY:CA	2:B:454:HOH:O	2.00	0.95
1:A:165:ARG:HG2	2:A:469:HOH:O	1.66	0.93
1:B:81:VAL:HG22	2:B:420:HOH:O	1.70	0.90
1:B:333:SER:HB3	2:B:416:HOH:O	1.73	0.88
1:B:264:SER:HA	2:B:414:HOH:O	1.74	0.85
1:A:340:PRO:CG	2:A:418:HOH:O	2.07	0.84
1:B:81:VAL:HG21	1:B:105:LYS:HA	1.58	0.83
1:B:165:ARG:HA	2:B:412:HOH:O	1.78	0.82
1:A:188:LEU:HD22	2:A:424:HOH:O	1.80	0.80
1:B:201:ARG:HG3	1:B:256:LEU:HD21	1.61	0.79
1:A:243:TYR:CB	2:A:411:HOH:O	2.24	0.79
1:A:201:ARG:HG3	1:A:256:LEU:HD21	1.66	0.77
1:A:166:GLY:HA2	1:A:169:PHE:HB2	1.68	0.74
1:A:340:PRO:CD	2:A:418:HOH:O	2.32	0.73
1:A:188:LEU:CD2	2:A:424:HOH:O	2.36	0.72
1:B:194:ASP:HA	1:B:197:LYS:HE2	1.71	0.71
1:A:124:TYR:HD2	1:A:223:LEU:HD11	1.56	0.70
1:B:61:LYS:HD3	1:B:66:ASN:HA	1.77	0.66
1:A:335:GLU:HB2	2:A:416:HOH:O	1.94	0.66
1:B:82:PHE:CD2	2:B:420:HOH:O	2.52	0.62
1:B:252:SER:OG	1:B:253:SEP:O1P	2.17	0.62
1:B:82:PHE:CE2	2:B:420:HOH:O	2.51	0.61
1:B:299:THR:C	2:B:417:HOH:O	2.39	0.60
1:A:64:THR:HG21	1:A:104:VAL:HG11	1.86	0.57
1:B:159:GLU:OE2	1:B:277:ARG:NH2	2.39	0.56
1:B:263:TYR:HD1	2:B:414:HOH:O	1.67	0.56
1:A:81:VAL:HG12	2:A:422:HOH:O	2.06	0.54
1:B:166:GLY:HA2	1:B:169:PHE:HB2	1.88	0.54
1:B:64:THR:HG21	1:B:104:VAL:HG11	1.90	0.53
1:A:252:SER:OG	1:A:253:SEP:O2P	2.23	0.51
1:B:141:LEU:HD23	1:B:146:ARG:HG2	1.93	0.51
1:B:299:THR:CA	2:B:417:HOH:O	2.59	0.51
1:B:279:LEU:HB2	2:B:454:HOH:O	2.10	0.51
1:A:176:LEU:HD21	1:B:176:LEU:HD21	1.93	0.50
1:B:161:HIS:HB3	1:B:172:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HB	1:A:104:VAL:O	2.13	0.49
1:A:57:PHE:O	1:A:61:LYS:HB2	2.13	0.48
1:A:109:GLN:O	2:A:401:HOH:O	2.20	0.48
1:A:161:HIS:HB3	1:A:172:LEU:HG	1.96	0.48
1:A:340:PRO:HD2	2:A:418:HOH:O	2.06	0.48
1:B:264:SER:CA	2:B:414:HOH:O	2.47	0.48
1:B:301:LYS:O	1:B:305:LEU:HD22	2.13	0.48
1:A:66:ASN:ND2	2:A:409:HOH:O	2.47	0.47
1:B:199:ILE:HD13	1:B:257:ASN:HA	1.96	0.47
1:A:58:ASN:HA	1:A:61:LYS:HB2	1.96	0.46
1:A:243:TYR:N	2:A:411:HOH:O	2.48	0.46
1:A:199:ILE:HD13	1:A:257:ASN:HA	1.97	0.46
1:B:124:TYR:HD2	1:B:223:LEU:HD11	1.81	0.46
1:A:292:ASP:OD1	1:A:295:ARG:NH2	2.44	0.46
1:B:183:ASP:HB2	1:B:216:ALA:HB3	1.98	0.46
1:A:105:LYS:HE3	1:A:107:LEU:HD21	1.97	0.45
1:A:135:LYS:HE3	1:A:137:ILE:HG12	1.97	0.45
1:A:171:PRO:HG3	1:A:311:ARG:CZ	2.47	0.45
1:A:82:PHE:HB2	1:A:104:VAL:CG1	2.47	0.45
1:A:81:VAL:CG1	2:A:422:HOH:O	2.63	0.44
1:B:82:PHE:HB2	1:B:104:VAL:CG1	2.47	0.44
1:B:263:TYR:C	2:B:414:HOH:O	2.56	0.44
1:B:82:PHE:HB2	1:B:104:VAL:HG13	1.98	0.44
1:B:165:ARG:CA	2:B:412:HOH:O	2.53	0.44
1:A:316:TYR:HA	2:A:413:HOH:O	2.16	0.44
1:A:140:CYS:HB3	1:A:147:LEU:HB2	1.99	0.44
1:B:243:TYR:HB3	2:B:410:HOH:O	2.17	0.44
1:A:81:VAL:HB	2:A:422:HOH:O	2.18	0.43
1:A:141:LEU:HA	1:A:145:HIS:O	2.18	0.43
1:B:351:GLN:NE2	1:B:355:ASN:OD1	2.51	0.43
1:A:137:ILE:N	1:A:149:VAL:O	2.44	0.43
1:B:166:GLY:N	2:B:412:HOH:O	2.51	0.43
1:B:171:PRO:HG3	1:B:311:ARG:CZ	2.48	0.42
1:A:298:LEU:HD13	1:A:329:VAL:HG22	2.02	0.42
1:A:341:THR:O	1:A:345:VAL:HG13	2.19	0.42
1:A:81:VAL:HG11	1:A:105:LYS:HA	2.01	0.42
1:B:298:LEU:HD13	1:B:329:VAL:HG22	2.02	0.41
1:A:155:LYS:HE3	1:A:214:TYR:CZ	2.56	0.41
1:A:116:ARG:CD	1:A:116:ARG:H	2.32	0.41
1:B:319:GLU:OE1	1:B:319:GLU:N	2.43	0.41
1:B:283:ARG:HG3	1:B:284:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LYS:HE3	1:B:214:TYR:CZ	2.56	0.41
1:B:264:SER:N	2:B:414:HOH:O	2.53	0.41
1:B:313:ASP:O	1:B:314:THR:OG1	2.29	0.40
1:B:58:ASN:HA	1:B:61:LYS:HB3	2.03	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	273/395 (69%)	255 (93%)	14 (5%)	4 (2%)	10 8
1	B	273/395 (69%)	254 (93%)	17 (6%)	2 (1%)	22 23
All	All	546/790 (69%)	509 (93%)	31 (6%)	6 (1%)	14 13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	B	164	ARG
1	A	165	ARG
1	A	81	VAL
1	B	81	VAL
1	A	166	GLY

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	243/339 (72%)	234 (96%)	9 (4%)	34	42
1	B	243/339 (72%)	237 (98%)	6 (2%)	47	58
All	All	486/678 (72%)	471 (97%)	15 (3%)	40	48

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	61	LYS
1	A	68	ARG
1	A	81	VAL
1	A	116	ARG
1	A	179	ASN
1	A	202	ASP
1	A	223	LEU
1	A	345	VAL
1	B	58	ASN
1	B	68	ARG
1	B	116	ARG
1	B	141	LEU
1	B	179	ASN
1	B	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	A	253	1	8,9,10	1.56	1 (12%)	8,12,14	1.57	2 (25%)
1	SEP	B	253	1	8,9,10	1.56	1 (12%)	8,12,14	1.57	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	253	1	-	0/5/8/10	-
1	SEP	B	253	1	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	SEP	P-O1P	3.44	1.61	1.50
1	B	253	SEP	P-O1P	3.39	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	SEP	OG-CB-CA	2.93	111.00	108.14
1	B	253	SEP	P-OG-CB	-2.90	110.30	118.30
1	B	253	SEP	OG-CB-CA	2.75	110.82	108.14
1	A	253	SEP	P-OG-CB	-2.64	111.02	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	253	SEP	1	0
1	B	253	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	279/395 (70%)	1.28	54 (19%) 1 2	30, 55, 87, 104	0
1	B	279/395 (70%)	1.34	58 (20%) 1 1	30, 56, 87, 98	0
All	All	558/790 (70%)	1.31	112 (20%) 1 2	30, 56, 87, 104	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	GLY	8.9
1	A	80	CYS	6.7
1	A	167	ALA	6.5
1	B	80	CYS	6.0
1	B	166	GLY	5.3
1	A	281	HIS	5.0
1	B	89	SER	4.9
1	B	284	PRO	4.7
1	A	282	ASN	4.4
1	A	223	LEU	4.3
1	A	284	PRO	4.3
1	A	89	SER	4.2
1	A	94	THR	4.1
1	B	288	GLU	4.1
1	B	360	SER	4.0
1	B	287	GLU	3.9
1	A	360	SER	3.8
1	A	52	VAL	3.8
1	B	281	HIS	3.7
1	B	167	ALA	3.6
1	A	98	THR	3.6
1	B	282	ASN	3.5
1	A	165	ARG	3.5
1	B	197	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	195	PRO	3.4
1	B	338	SER	3.4
1	B	66	ASN	3.4
1	B	193	SER	3.4
1	B	168	TYR	3.3
1	A	163	PHE	3.3
1	A	285	ALA	3.3
1	B	163	PHE	3.3
1	B	81	VAL	3.2
1	B	94	THR	3.1
1	A	243	TYR	3.1
1	B	333	SER	3.1
1	B	223	LEU	3.1
1	B	181	ALA	3.0
1	A	333	SER	3.0
1	A	124	TYR	3.0
1	B	123	ASN	2.9
1	B	293	TRP	2.8
1	A	287	GLU	2.8
1	B	201	ARG	2.8
1	A	335	GLU	2.8
1	B	196	VAL	2.8
1	B	107	LEU	2.8
1	B	124	TYR	2.7
1	B	334	PHE	2.7
1	A	256	LEU	2.7
1	B	178	VAL	2.7
1	B	222	GLY	2.7
1	A	296	PRO	2.7
1	A	197	LYS	2.6
1	A	279	LEU	2.6
1	A	172	LEU	2.6
1	A	194	ASP	2.6
1	B	158	LEU	2.6
1	B	165	ARG	2.6
1	B	82	PHE	2.6
1	B	62	LEU	2.6
1	A	168	TYR	2.6
1	A	123	ASN	2.6
1	A	193	SER	2.5
1	A	158	LEU	2.5
1	B	348	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	106	LYS	2.5
1	B	182	LEU	2.5
1	A	251	MET	2.5
1	B	116	ARG	2.5
1	B	296	PRO	2.5
1	A	180	VAL	2.5
1	A	344	GLN	2.4
1	A	143	ASP	2.4
1	A	280	ASP	2.4
1	B	175	PHE	2.4
1	B	327	VAL	2.4
1	A	182	LEU	2.4
1	B	324	MET	2.4
1	A	258	ALA	2.3
1	B	335	GLU	2.3
1	B	98	THR	2.3
1	B	344	GLN	2.3
1	A	144	GLU	2.3
1	B	147	LEU	2.3
1	B	285	ALA	2.3
1	A	322	VAL	2.3
1	A	135	LYS	2.3
1	A	195	PRO	2.3
1	B	349	LEU	2.2
1	A	324	MET	2.2
1	B	110	GLU	2.2
1	B	359	PRO	2.2
1	A	349	LEU	2.2
1	A	196	VAL	2.2
1	B	142	GLU	2.2
1	B	180	VAL	2.2
1	A	181	ALA	2.2
1	B	67	PHE	2.1
1	A	332	LEU	2.1
1	B	243	TYR	2.1
1	B	93	PRO	2.1
1	A	175	PHE	2.1
1	A	327	VAL	2.1
1	A	67	PHE	2.1
1	B	69	PRO	2.1
1	A	82	PHE	2.0
1	A	107	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	99	GLY	2.0
1	A	185	ALA	2.0
1	A	326	SER	2.0
1	B	289	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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
1	SEP	A	253	10/11	0.91	0.21	73,77,87,95	0
1	SEP	B	253	10/11	0.92	0.21	73,77,87,87	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.