



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:55 PM UTC

PDB ID : 5W85 / pdb_00005w85
Title : CRYSTAL STRUCTURE OF IRAK-4 WITH A 4,6-DIAMINONICOTINAMIDE INHIBITOR (COMPOUND NUMBER 9)
Authors : Sack, J.S.
Deposited on : 2017-06-21
Resolution : 2.25 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

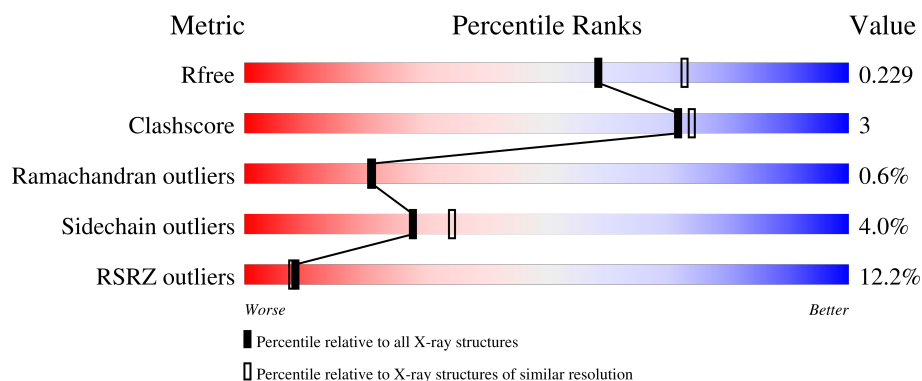
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	305	9% 80% 11% 8%
1	B	305	14% 78% 13% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4586 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.

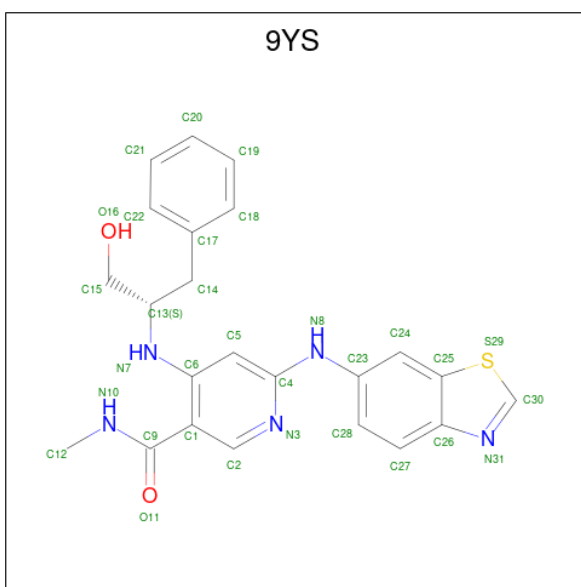
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	P	S	0	0	0
			2216	1390	370	439	3	14			
1	B	282	Total	C	N	O	P	S	0	0	0
			2201	1376	371	437	3	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q9NWZ3
A	157	ALA	-	expression tag	UNP Q9NWZ3
A	158	MET	-	expression tag	UNP Q9NWZ3
A	159	GLY	-	expression tag	UNP Q9NWZ3
B	156	GLY	-	expression tag	UNP Q9NWZ3
B	157	ALA	-	expression tag	UNP Q9NWZ3
B	158	MET	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 6-[(1,3-benzothiazol-6-yl)amino]-4-[[[(2S)-1-hydroxy-3-phenylpropan-2-yl]amino]-N-methylpyridine-3-carboxamide (CCD ID: 9YS) (formula: C₂₃H₂₃N₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	23	5	2	1		
2	B	1	Total	C	N	O	S	0	0
			31	23	5	2	1		

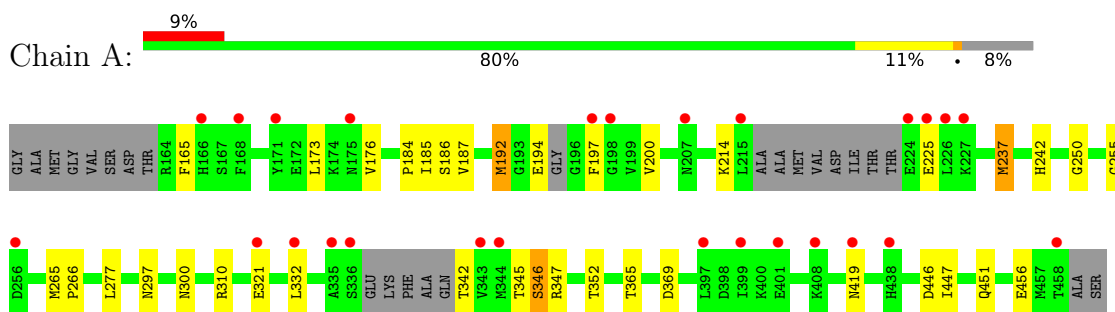
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		
3	B	48	Total	O	0	0
			48	48		

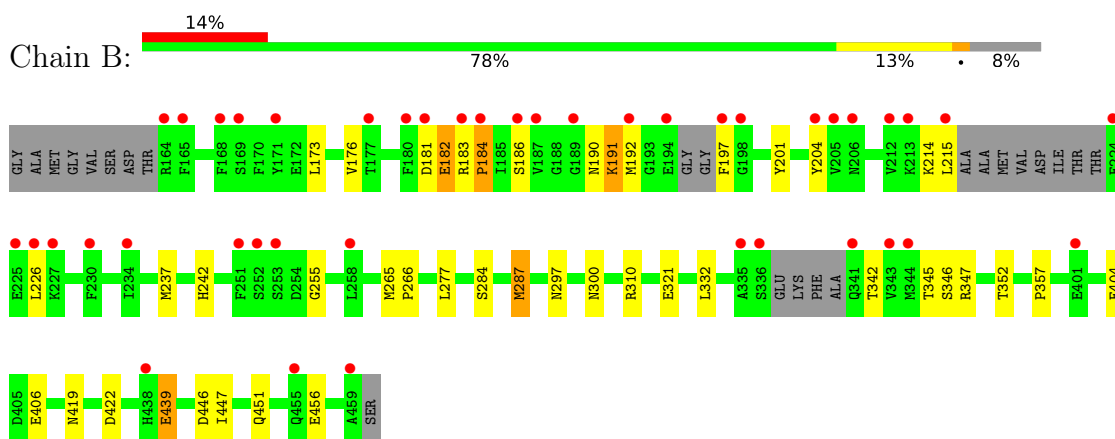
3 Residue-property plots

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: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	88.44Å 125.56Å 141.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.25 29.72 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.72-2.25) 94.0 (29.72-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.227 , 0.251 0.217 , 0.229	Depositor DCC
R_{free} test set	780 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4586	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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 41.73 % 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 2.2624e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9YS, SEP, TPO

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	0.85	2/2218 (0.1%)	1.31	16/2986 (0.5%)
1	B	0.84	2/2201 (0.1%)	1.28	11/2964 (0.4%)
All	All	0.84	4/4419 (0.1%)	1.30	27/5950 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	MET	SD-CE	-8.11	1.59	1.79
1	B	287	MET	SD-CE	-6.65	1.62	1.79
1	B	265	MET	SD-CE	-6.06	1.64	1.79
1	A	192	MET	SD-CE	-5.99	1.64	1.79

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	PHE	CA-CB-CG	-7.99	105.81	113.80
1	A	185	ILE	CA-C-N	5.64	128.62	120.38
1	A	185	ILE	C-N-CA	5.64	128.62	120.38
1	A	255	GLY	CA-C-N	5.62	128.12	120.54
1	A	255	GLY	C-N-CA	5.62	128.12	120.54
1	B	255	GLY	CA-C-N	5.55	128.03	120.54
1	B	255	GLY	C-N-CA	5.55	128.03	120.54
1	A	197	PHE	CA-C-N	5.49	129.36	121.56
1	A	197	PHE	C-N-CA	5.49	129.36	121.56
1	A	446	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	446	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	242	HIS	CA-C-N	5.47	128.16	120.28
1	A	242	HIS	C-N-CA	5.47	128.16	120.28
1	B	242	HIS	CA-C-N	5.46	128.15	120.28
1	B	242	HIS	C-N-CA	5.46	128.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	PRO	CA-C-N	5.46	128.23	120.53
1	A	184	PRO	C-N-CA	5.46	128.23	120.53
1	A	456	GLU	CA-C-N	5.27	127.34	120.28
1	A	456	GLU	C-N-CA	5.27	127.34	120.28
1	A	369	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	422	ASP	CA-C-N	5.11	127.37	120.38
1	B	422	ASP	C-N-CA	5.11	127.37	120.38
1	B	456	GLU	CA-C-N	5.11	127.12	120.28
1	B	456	GLU	C-N-CA	5.11	127.12	120.28
1	B	197	PHE	CA-C-N	5.03	126.03	122.16
1	B	197	PHE	C-N-CA	5.03	126.03	122.16
1	A	225	GLU	N-CA-C	-5.01	107.22	113.38

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	2216	0	2172	11	0
1	B	2201	0	2138	18	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
3	A	59	0	0	0	0
3	B	48	0	0	0	0
All	All	4586	0	4310	29	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 (29) 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:183:ARG:O	1:B:191:LYS:HB3	1.78	0.84
1:B:284:SER:H	1:B:287:MET:HE3	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:HD22	1:A:451:GLN:HE21	1.44	0.66
1:B:297:ASN:HD22	1:B:451:GLN:HE21	1.49	0.61
1:B:266:PRO:HG2	1:B:321:GLU:HG3	1.85	0.57
1:B:357:PRO:HG3	1:B:439:GLU:HG2	1.87	0.56
1:A:297:ASN:ND2	1:A:451:GLN:HE21	2.05	0.55
1:A:310:ARG:HD3	1:A:332:LEU:O	2.10	0.52
1:B:297:ASN:ND2	1:B:451:GLN:HE21	2.08	0.51
1:A:266:PRO:HG2	1:A:321:GLU:HG3	1.92	0.50
1:A:173:LEU:HA	1:A:176:VAL:HG22	1.93	0.50
1:B:176:VAL:HG22	1:B:204:TYR:H	1.76	0.49
1:B:310:ARG:HD3	1:B:332:LEU:O	2.11	0.49
1:B:183:ARG:O	1:B:191:LYS:N	2.45	0.48
1:A:192:MET:HE3	1:A:200:VAL:HG12	1.95	0.47
1:B:173:LEU:HA	1:B:176:VAL:HG12	1.97	0.46
1:A:321:GLU:H	1:A:321:GLU:CD	2.24	0.46
1:B:183:ARG:CB	1:B:184:PRO:HD3	2.46	0.46
1:B:321:GLU:H	1:B:321:GLU:CD	2.25	0.45
1:B:215:LEU:HB3	1:B:226:LEU:HD23	1.99	0.44
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.99	0.43
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.00	0.42
1:B:190:ASN:O	1:B:201:TYR:HA	2.20	0.42
1:A:165:PHE:HB3	1:A:250:GLY:HA2	2.02	0.42
1:A:346:SEP:O	1:A:347:ARG:HB3	2.21	0.41
1:B:284:SER:H	1:B:287:MET:CE	2.23	0.41
1:A:237:MET:HA	1:A:237:MET:HE2	2.03	0.40
1:B:181:ASP:C	1:B:183:ARG:H	2.28	0.40
1:B:404:GLU:C	1:B:406:GLU:H	2.30	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	271/305 (89%)	261 (96%)	10 (4%)	0	100	100
1	B	271/305 (89%)	259 (96%)	9 (3%)	3 (1%)	11	8
All	All	542/610 (89%)	520 (96%)	19 (4%)	3 (1%)	21	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	347	ARG
1	B	182	GLU
1	B	184	PRO

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	241/260 (93%)	232 (96%)	9 (4%)	30	37
1	B	236/260 (91%)	226 (96%)	10 (4%)	26	31
All	All	477/520 (92%)	458 (96%)	19 (4%)	28	34

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	SER
1	A	187	VAL
1	A	194	GLU
1	A	214	LYS
1	A	237	MET
1	A	277	LEU
1	A	352	THR
1	A	365	THR
1	A	419	ASN
1	B	182	GLU
1	B	186	SER
1	B	191	LYS
1	B	192	MET

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Mol	Chain	Res	Type
1	B	214	LYS
1	B	237	MET
1	B	277	LEU
1	B	352	THR
1	B	419	ASN
1	B	439	GLU

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	178	ASN
1	A	190	ASN
1	A	232	GLN
1	A	244	ASN
1	A	297	ASN
1	A	300	ASN
1	A	305	ASN
1	A	435	GLN
1	A	442	ASN
1	A	451	GLN
1	B	166	HIS
1	B	190	ASN
1	B	232	GLN
1	B	244	ASN
1	B	286	HIS
1	B	297	ASN
1	B	300	ASN
1	B	390	HIS
1	B	435	GLN
1	B	442	ASN
1	B	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	TPO	B	342	1	8,10,11	1.09	1 (12%)	10,14,16	1.36	2 (20%)
1	TPO	A	345	1	8,10,11	1.92	3 (37%)	10,14,16	1.13	1 (10%)
1	SEP	B	346	1	8,9,10	0.93	0	7,12,14	2.19	2 (28%)
1	TPO	A	342	1	8,10,11	1.04	0	10,14,16	1.43	2 (20%)
1	SEP	A	346	1	8,9,10	1.04	0	7,12,14	1.30	1 (14%)
1	TPO	B	345	1	8,10,11	1.42	1 (12%)	10,14,16	1.39	3 (30%)

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	TPO	B	342	1	-	1/9/11/13	-
1	TPO	A	345	1	-	2/9/11/13	-
1	SEP	B	346	1	-	5/6/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	P-OG1	-3.34	1.53	1.59
1	A	345	TPO	CB-CA	3.18	1.60	1.53
1	B	345	TPO	CB-CA	2.91	1.60	1.53
1	A	345	TPO	CG2-CB	2.32	1.57	1.51
1	B	342	TPO	P-OG1	-2.13	1.55	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-CB-CA	4.08	112.12	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	O2P-P-OG	3.77	116.50	106.67
1	A	346	SEP	O3P-P-OG	3.19	115.00	106.67
1	A	342	TPO	O2P-P-OG1	3.03	117.64	105.85
1	B	342	TPO	O2P-P-OG1	2.95	117.36	105.85
1	B	345	TPO	O2P-P-OG1	2.58	115.89	105.85
1	A	342	TPO	P-OG1-CB	-2.56	116.37	123.33
1	B	342	TPO	P-OG1-CB	-2.43	116.71	123.33
1	A	345	TPO	O3P-P-OG1	2.31	114.86	105.85
1	B	345	TPO	CG2-CB-CA	2.04	117.23	113.26
1	B	345	TPO	P-OG1-CB	-2.01	117.85	123.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	346	SEP	N-CA-CB-OG
1	B	346	SEP	CB-OG-P-O1P
1	B	346	SEP	CB-OG-P-O2P
1	B	346	SEP	CB-OG-P-O3P
1	B	346	SEP	CA-CB-OG-P
1	B	345	TPO	CA-CB-OG1-P
1	A	342	TPO	C-CA-CB-CG2
1	A	345	TPO	O-C-CA-CB
1	B	342	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	346	SEP	1	0

5.5 Carbohydrates

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	9YS	A	4000	-	34,34,34	0.29	0	42,46,46	0.62	0
2	9YS	B	4000	-	34,34,34	0.26	0	42,46,46	0.61	0

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
2	9YS	A	4000	-	-	0/20/20/20	0/4/4/4
2	9YS	B	4000	-	-	0/20/20/20	0/4/4/4

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	278/305 (91%)	0.61	26 (9%) 14 13	36, 57, 93, 105	0
1	B	279/305 (91%)	0.87	42 (15%) 5 5	39, 63, 116, 133	0
All	All	557/610 (91%)	0.74	68 (12%) 8 8	36, 59, 108, 133	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	459	ALA	5.7
1	B	197	PHE	5.1
1	B	181	ASP	4.5
1	B	335	ALA	4.4
1	B	230	PHE	4.2
1	A	399	ILE	4.1
1	B	226	LEU	3.9
1	B	215	LEU	3.9
1	B	165	PHE	3.8
1	B	198	GLY	3.7
1	B	251	PHE	3.6
1	A	226	LEU	3.6
1	B	183	ARG	3.5
1	B	192	MET	3.4
1	A	343	VAL	3.4
1	A	168	PHE	3.3
1	A	344	MET	3.2
1	B	187	VAL	3.2
1	B	204	TYR	3.1
1	B	213	LYS	3.1
1	A	332	LEU	3.0
1	B	171	TYR	3.0
1	B	224	GLU	3.0
1	B	341	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	2.9
1	B	180	PHE	2.9
1	B	194	GLU	2.9
1	B	253	SER	2.9
1	A	197	PHE	2.9
1	A	458	THR	2.9
1	B	401	GLU	2.8
1	A	224	GLU	2.8
1	A	215	LEU	2.7
1	B	225	GLU	2.7
1	A	256	ASP	2.7
1	B	206	ASN	2.6
1	B	184	PRO	2.4
1	B	177	THR	2.4
1	A	336	SER	2.4
1	A	166	HIS	2.4
1	A	419	ASN	2.4
1	A	198	GLY	2.4
1	B	227	LYS	2.4
1	A	401	GLU	2.3
1	A	408	LYS	2.2
1	A	171	TYR	2.2
1	B	336	SER	2.2
1	B	164	ARG	2.2
1	B	344	MET	2.2
1	B	189	GLY	2.2
1	B	258	LEU	2.2
1	B	455	GLN	2.2
1	B	252	SER	2.2
1	A	175	ASN	2.1
1	B	212	VAL	2.1
1	A	207	ASN	2.1
1	A	321	GLU	2.1
1	A	438	HIS	2.1
1	B	205	VAL	2.1
1	B	168	PHE	2.1
1	B	186	SER	2.1
1	B	438	HIS	2.1
1	A	227	LYS	2.0
1	A	225	GLU	2.0
1	A	397	LEU	2.0
1	B	234	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	169	SER	2.0
1	A	335	ALA	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, 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
1	SEP	A	346	10/11	0.69	0.14	84,90,98,98	0
1	SEP	B	346	10/11	0.74	0.11	88,93,101,102	0
1	TPO	A	342	11/12	0.80	0.17	96,98,104,105	0
1	TPO	B	342	11/12	0.84	0.15	100,102,105,105	0
1	TPO	B	345	11/12	0.94	0.10	83,86,87,89	0
1	TPO	A	345	11/12	0.94	0.10	81,83,83,85	0

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(Å ²)	Q<0.9
2	9YS	B	4000	31/31	0.92	0.10	54,60,68,69	0
2	9YS	A	4000	31/31	0.96	0.06	40,46,53,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.