



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 09:52 pm BST

PDB ID : 3TL8
Title : The AvrPtoB-BAK1 complex reveals two structurally similar kinase interacting domains in a single type III effector
Authors : Chai, J.; Cheng, W.; Gao, H.
Deposited on : 2011-08-29
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

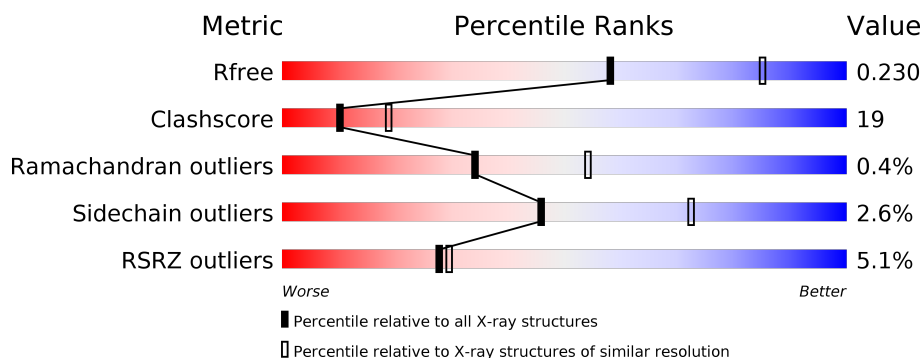
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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 $\leq 5\%$. 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	349	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>30%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	349	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>26%</div> <div>•</div> <div>11%</div> </div> </div>
1	G	349	<div> <div>7%</div> <div> <div></div> <div>61%</div> <div>25%</div> <div>•</div> <div>13%</div> </div> </div>
1	H	349	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>•</div> <div>12%</div> </div> </div>
2	B	117	<div> <div>7%</div> <div> <div></div> <div>43%</div> <div>31%</div> <div>•</div> <div>26%</div> </div> </div>
2	F	117	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>25%</div> <div></div> <div>25%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	K	117	
2	L	117	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	D	324	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12644 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 BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	P	S	0	0	0
			2422	1516	426	462	4	14			
1	D	310	Total	C	N	O	P	S	0	0	0
			2475	1550	436	470	4	15			
1	G	305	Total	C	N	O	P	S	0	0	0
			2435	1524	427	466	4	14			
1	H	307	Total	C	N	O	P	S	0	0	0
			2448	1532	429	468	4	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	591	LEU	-	EXPRESSION TAG	UNP Q94F62
A	592	GLU	-	EXPRESSION TAG	UNP Q94F62
A	593	HIS	-	EXPRESSION TAG	UNP Q94F62
A	594	HIS	-	EXPRESSION TAG	UNP Q94F62
A	595	HIS	-	EXPRESSION TAG	UNP Q94F62
A	596	HIS	-	EXPRESSION TAG	UNP Q94F62
A	597	HIS	-	EXPRESSION TAG	UNP Q94F62
A	598	HIS	-	EXPRESSION TAG	UNP Q94F62
D	591	LEU	-	EXPRESSION TAG	UNP Q94F62
D	592	GLU	-	EXPRESSION TAG	UNP Q94F62
D	593	HIS	-	EXPRESSION TAG	UNP Q94F62
D	594	HIS	-	EXPRESSION TAG	UNP Q94F62
D	595	HIS	-	EXPRESSION TAG	UNP Q94F62
D	596	HIS	-	EXPRESSION TAG	UNP Q94F62
D	597	HIS	-	EXPRESSION TAG	UNP Q94F62
D	598	HIS	-	EXPRESSION TAG	UNP Q94F62
G	591	LEU	-	EXPRESSION TAG	UNP Q94F62
G	592	GLU	-	EXPRESSION TAG	UNP Q94F62
G	593	HIS	-	EXPRESSION TAG	UNP Q94F62
G	594	HIS	-	EXPRESSION TAG	UNP Q94F62

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Chain	Residue	Modelled	Actual	Comment	Reference
G	595	HIS	-	EXPRESSION TAG	UNP Q94F62
G	596	HIS	-	EXPRESSION TAG	UNP Q94F62
G	597	HIS	-	EXPRESSION TAG	UNP Q94F62
G	598	HIS	-	EXPRESSION TAG	UNP Q94F62
H	591	LEU	-	EXPRESSION TAG	UNP Q94F62
H	592	GLU	-	EXPRESSION TAG	UNP Q94F62
H	593	HIS	-	EXPRESSION TAG	UNP Q94F62
H	594	HIS	-	EXPRESSION TAG	UNP Q94F62
H	595	HIS	-	EXPRESSION TAG	UNP Q94F62
H	596	HIS	-	EXPRESSION TAG	UNP Q94F62
H	597	HIS	-	EXPRESSION TAG	UNP Q94F62
H	598	HIS	-	EXPRESSION TAG	UNP Q94F62

- Molecule 2 is a protein called Effector protein HopAB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			664	408	133	120	3			
2	F	88	Total	C	N	O	S	0	0	0
			672	414	134	121	3			
2	K	88	Total	C	N	O	S	0	0	0
			676	416	134	123	3			
2	L	87	Total	C	N	O	S	0	0	0
			664	408	133	120	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	243	GLY	-	SEE REMARK 999	UNP Q8RSY1
B	244	PRO	-	SEE REMARK 999	UNP Q8RSY1
B	245	LEU	-	SEE REMARK 999	UNP Q8RSY1
B	246	GLY	-	SEE REMARK 999	UNP Q8RSY1
B	247	SER	-	SEE REMARK 999	UNP Q8RSY1
F	243	GLY	-	SEE REMARK 999	UNP Q8RSY1
F	244	PRO	-	SEE REMARK 999	UNP Q8RSY1
F	245	LEU	-	SEE REMARK 999	UNP Q8RSY1
F	246	GLY	-	SEE REMARK 999	UNP Q8RSY1
F	247	SER	-	SEE REMARK 999	UNP Q8RSY1
K	243	GLY	-	SEE REMARK 999	UNP Q8RSY1
K	244	PRO	-	SEE REMARK 999	UNP Q8RSY1
K	245	LEU	-	SEE REMARK 999	UNP Q8RSY1
K	246	GLY	-	SEE REMARK 999	UNP Q8RSY1

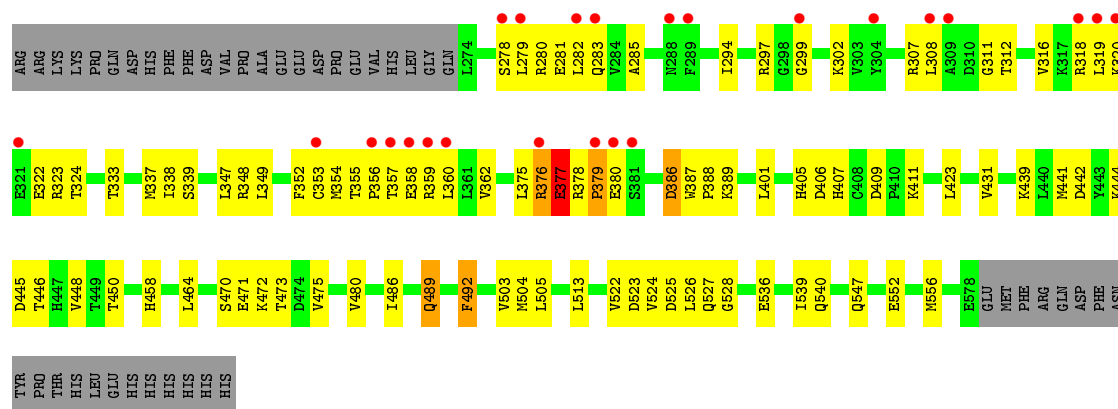
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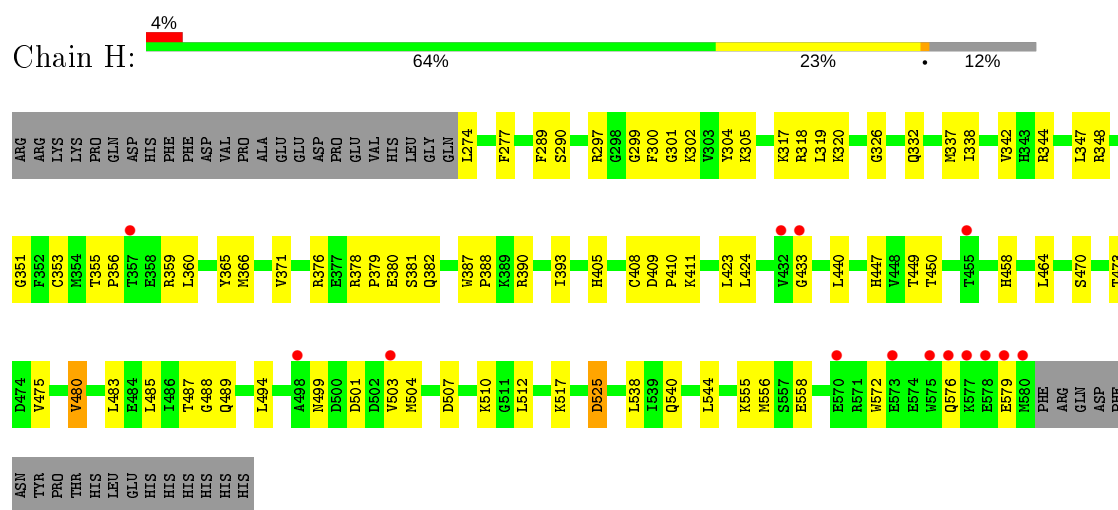
Chain	Residue	Modelled	Actual	Comment	Reference
K	247	SER	-	SEE REMARK 999	UNP Q8RSY1
L	243	GLY	-	SEE REMARK 999	UNP Q8RSY1
L	244	PRO	-	SEE REMARK 999	UNP Q8RSY1
L	245	LEU	-	SEE REMARK 999	UNP Q8RSY1
L	246	GLY	-	SEE REMARK 999	UNP Q8RSY1
L	247	SER	-	SEE REMARK 999	UNP Q8RSY1

- Molecule 3 is water.

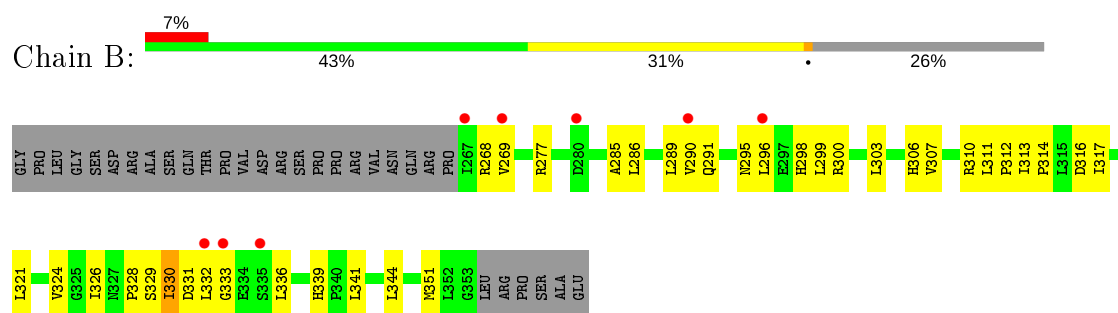
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	9	Total O 9 9	0	0
3	D	38	Total O 38 38	0	0
3	F	9	Total O 9 9	0	0
3	G	34	Total O 34 34	0	0
3	H	33	Total O 33 33	0	0
3	K	9	Total O 9 9	0	0
3	L	10	Total O 10 10	0	0



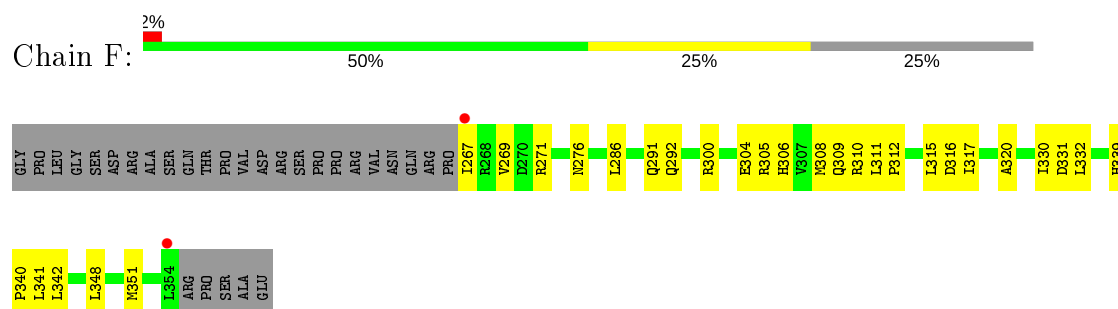
- Molecule 1: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1



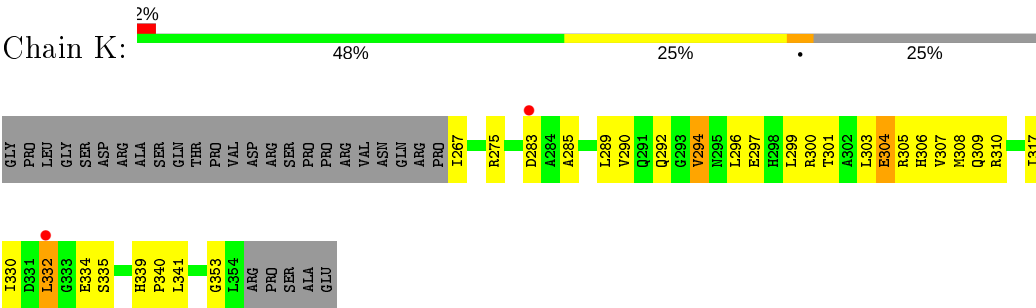
- Molecule 2: Effector protein HopAB2



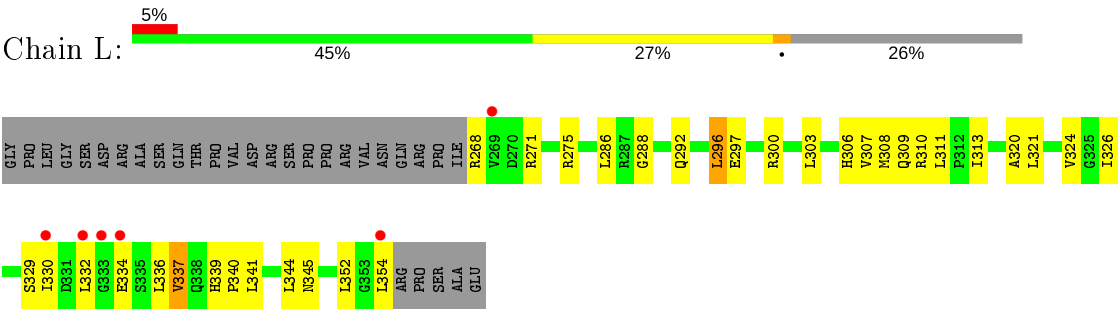
- Molecule 2: Effector protein HopAB2



● Molecule 2: Effector protein HopAB2



● Molecule 2: Effector protein HopAB2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.84Å 108.14Å 83.25Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	24.14 – 2.50 45.33 – 2.47	Depositor EDS
% Data completeness (in resolution range)	97.4 (24.14-2.50) 96.6 (45.33-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.184 , 0.238 0.179 , 0.230	Depositor DCC
R_{free} test set	3323 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.007 for -k,-h,-l 0.012 for k,h,-l 0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12644	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/2415	0.55	1/3247 (0.0%)
1	D	0.44	1/2469 (0.0%)	0.57	0/3317
1	G	0.46	0/2428	0.60	2/3263 (0.1%)
1	H	0.38	0/2441	0.53	1/3280 (0.0%)
2	B	0.29	0/670	0.52	0/907
2	F	0.48	0/678	0.53	0/918
2	K	0.57	0/682	0.58	0/923
2	L	0.55	0/670	0.57	0/907
All	All	0.44	1/12453 (0.0%)	0.56	4/16762 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	374	CYS	CB-SG	-5.42	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	377	GLU	N-CA-CB	13.59	135.05	110.60
1	H	433	GLY	N-CA-C	5.64	127.20	113.10
1	G	376	ARG	N-CA-C	-5.44	96.31	111.00
1	A	433	GLY	N-CA-C	5.07	125.78	113.10

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	2422	0	2420	100	3
1	D	2475	0	2471	94	3
1	G	2435	0	2433	91	0
1	H	2448	0	2445	74	0
2	B	664	0	686	48	0
2	F	672	0	697	27	0
2	K	676	0	701	46	0
2	L	664	0	686	46	0
3	A	46	0	0	1	0
3	B	9	0	0	1	0
3	D	38	0	0	0	0
3	F	9	0	0	0	0
3	G	34	0	0	1	0
3	H	33	0	0	1	0
3	K	9	0	0	0	0
3	L	10	0	0	1	0
All	All	12644	0	12539	471	3

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 19.

The worst 5 of 471 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:D:376:ARG:HH12	1:D:489:GLN:CD	1.03	1.47
1:H:504:MET:HG2	2:L:309:GLN:NE2	1.49	1.27
1:D:376:ARG:NH1	1:D:489:GLN:CD	1.88	1.25
1:D:355:THR:HB	1:D:356:PRO:HD2	1.22	1.17
1:H:504:MET:CG	2:L:309:GLN:HE22	1.58	1.15

All (3) 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:A:280:ARG:NE	1:D:583:GLN:OE1[2_546]	1.03	1.17
1:A:280:ARG:CZ	1:D:583:GLN:OE1[2_546]	1.82	0.38
1:A:496:ARG:NH1	1:D:502:ASP:OD1[1_554]	2.09	0.11

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	298/349 (85%)	286 (96%)	11 (4%)	1 (0%)	41	61
1	D	304/349 (87%)	292 (96%)	11 (4%)	1 (0%)	41	61
1	G	299/349 (86%)	279 (93%)	17 (6%)	3 (1%)	15	28
1	H	301/349 (86%)	289 (96%)	12 (4%)	0	100	100
2	B	85/117 (73%)	81 (95%)	3 (4%)	1 (1%)	13	24
2	F	86/117 (74%)	84 (98%)	2 (2%)	0	100	100
2	K	86/117 (74%)	83 (96%)	3 (4%)	0	100	100
2	L	85/117 (73%)	82 (96%)	3 (4%)	0	100	100
All	All	1544/1864 (83%)	1476 (96%)	62 (4%)	6 (0%)	34	54

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	377	GLU
1	G	379	PRO
2	B	330	ILE
1	G	356	PRO
1	A	376	ARG

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	254/298 (85%)	247 (97%)	7 (3%)	43	70
1	D	259/298 (87%)	250 (96%)	9 (4%)	36	62
1	G	256/298 (86%)	252 (98%)	4 (2%)	62	84
1	H	257/298 (86%)	253 (98%)	4 (2%)	62	84
2	B	71/98 (72%)	70 (99%)	1 (1%)	67	86
2	F	72/98 (74%)	72 (100%)	0	100	100
2	K	73/98 (74%)	69 (94%)	4 (6%)	21	41
2	L	71/98 (72%)	66 (93%)	5 (7%)	15	29
All	All	1313/1584 (83%)	1279 (97%)	34 (3%)	46	72

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	515	GLU
1	G	489	GLN
2	L	329	SER
1	G	386	ASP
1	A	575	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	489	GLN
1	H	283	GLN
2	L	339	HIS
1	G	499	ASN
1	G	540	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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	H	450	1	8,10,11	0.79	0	10,14,16	0.92	0
1	TPO	D	324	1	8,10,11	0.84	0	10,14,16	1.19	1 (10%)
1	TPO	A	324	1	8,10,11	1.25	1 (12%)	10,14,16	1.18	1 (10%)
1	TPO	D	449	1	8,10,11	0.93	0	10,14,16	0.95	1 (10%)
1	TPO	H	446	1	8,10,11	0.96	0	10,14,16	0.96	0
1	TPO	D	450	1	8,10,11	0.93	0	10,14,16	0.91	0
1	TPO	D	446	1	8,10,11	1.18	0	10,14,16	1.03	0
1	TPO	A	449	1	8,10,11	1.06	0	10,14,16	1.00	0
1	TPO	G	446	1	8,10,11	1.05	0	10,14,16	1.50	2 (20%)
1	TPO	G	449	1	8,10,11	0.88	0	10,14,16	0.90	0
1	TPO	A	446	1	8,10,11	1.09	0	10,14,16	1.12	0
1	TPO	A	450	1	8,10,11	0.73	0	10,14,16	1.00	1 (10%)
1	TPO	H	449	1	8,10,11	0.96	0	10,14,16	0.90	0
1	TPO	G	450	1	8,10,11	0.87	0	10,14,16	0.81	0
1	TPO	H	324	1	8,10,11	1.24	0	10,14,16	1.06	0
1	TPO	G	324	1	8,10,11	1.04	0	10,14,16	0.99	1 (10%)

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	H	450	1	-	5/9/11/13	-
1	TPO	D	324	1	-	4/9/11/13	-
1	TPO	A	324	1	-	1/9/11/13	-
1	TPO	D	449	1	-	2/9/11/13	-
1	TPO	H	446	1	-	0/9/11/13	-
1	TPO	D	450	1	-	5/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	D	446	1	-	1/9/11/13	-
1	TPO	A	449	1	-	1/9/11/13	-
1	TPO	G	446	1	-	4/9/11/13	-
1	TPO	G	449	1	-	2/9/11/13	-
1	TPO	A	446	1	-	1/9/11/13	-
1	TPO	A	450	1	-	5/9/11/13	-
1	TPO	H	449	1	-	2/9/11/13	-
1	TPO	G	450	1	-	3/9/11/13	-
1	TPO	H	324	1	-	2/9/11/13	-
1	TPO	G	324	1	-	5/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	TPO	P-OG1	-2.34	1.54	1.59

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	446	TPO	CB-CA-N	-2.72	96.52	114.41
1	G	446	TPO	CG2-CB-CA	-2.52	108.18	113.16
1	A	324	TPO	P-OG1-CB	-2.52	115.60	123.21
1	D	324	TPO	P-OG1-CB	-2.29	116.31	123.21
1	A	450	TPO	O-C-CA	-2.17	119.10	124.78

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	450	TPO	N-CA-CB-OG1
1	H	450	TPO	CA-CB-OG1-P
1	H	450	TPO	CB-OG1-P-O3P
1	D	324	TPO	O-C-CA-CB
1	D	324	TPO	CG2-CB-OG1-P

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	450	TPO	3	0
1	D	324	TPO	6	0
1	A	449	TPO	1	0
1	G	446	TPO	2	0
1	A	446	TPO	1	0
1	H	449	TPO	1	0
1	G	450	TPO	1	0
1	G	324	TPO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	300/349 (85%)	0.22	9 (3%) 50 53	24, 58, 101, 134	0
1	D	306/349 (87%)	0.27	14 (4%) 32 34	24, 54, 101, 133	0
1	G	301/349 (86%)	0.51	24 (7%) 12 12	26, 62, 114, 152	0
1	H	303/349 (86%)	0.31	14 (4%) 32 34	25, 53, 105, 143	0
2	B	87/117 (74%)	0.76	8 (9%) 9 9	42, 79, 114, 128	0
2	F	88/117 (75%)	-0.00	2 (2%) 60 63	28, 50, 95, 108	0
2	K	88/117 (75%)	-0.10	2 (2%) 60 63	36, 64, 97, 126	0
2	L	87/117 (74%)	0.27	6 (6%) 16 17	37, 63, 92, 144	0
All	All	1560/1864 (83%)	0.30	79 (5%) 28 29	24, 59, 106, 152	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	332	LEU	6.3
1	G	319	LEU	5.0
1	H	575	TRP	4.7
1	D	577	LYS	4.6
2	B	296	LEU	4.5

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	TPO	G	324	11/12	0.92	0.15	57,84,95,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TPO	D	324	11/12	0.95	0.13	44,58,157,160	0
1	TPO	G	446	11/12	0.96	0.09	46,57,75,81	0
1	TPO	G	449	11/12	0.96	0.13	30,37,51,66	0
1	TPO	A	446	11/12	0.96	0.12	51,62,90,95	0
1	TPO	A	324	11/12	0.96	0.11	61,67,74,75	0
1	TPO	H	446	11/12	0.97	0.10	51,56,77,81	0
1	TPO	H	449	11/12	0.97	0.11	26,42,63,70	0
1	TPO	H	324	11/12	0.97	0.11	63,74,80,86	0
1	TPO	D	446	11/12	0.97	0.12	56,68,84,85	0
1	TPO	D	449	11/12	0.99	0.11	35,43,59,68	0
1	TPO	A	450	11/12	0.99	0.14	16,36,45,46	0
1	TPO	A	449	11/12	0.99	0.08	33,45,61,67	0
1	TPO	G	450	11/12	0.99	0.14	14,31,36,39	0
1	TPO	H	450	11/12	0.99	0.13	27,34,40,40	0
1	TPO	D	450	11/12	0.99	0.12	18,31,36,40	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.