



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2020 – 04:24 PM EST

PDB ID : 6W3C
Title : Structure of phosphorylated apo IRE1
Authors : Wallweber, H.; Mortara, K.; Ferri, E.; Wang, W.; Rudolph, J.
Deposited on : 2020-03-09
Resolution : 2.30 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 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 : 2.14.6
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) : 2.14.6

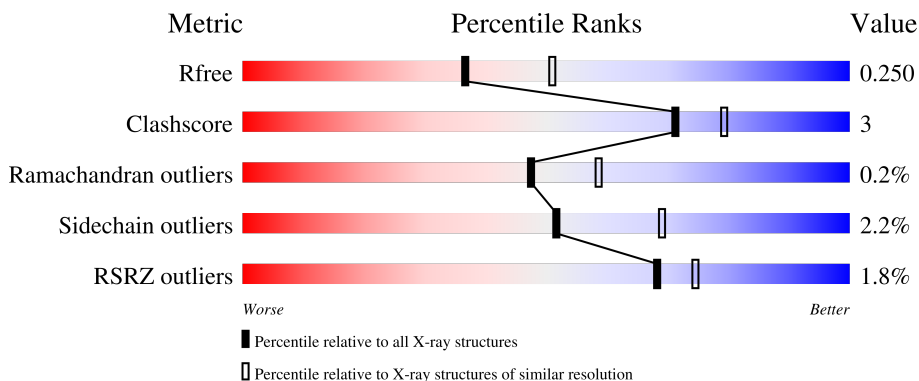
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	434	<div> <div>0%</div> <div>82% 10% • 7%</div> </div>
1	B	434	<div> <div>2%</div> <div>82% 10% • 7%</div> </div>
1	C	434	<div> <div>3%</div> <div>81% 11% • 7%</div> </div>
1	D	434	<div> <div></div> <div>85% 7% • 7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13478 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/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	P	S	0	0	0
			3285	2083	582	597	3	20			
1	B	404	Total	C	N	O	P	S	0	0	0
			3280	2080	581	596	3	20			
1	C	404	Total	C	N	O	P	S	0	0	0
			3280	2080	581	596	3	20			
1	D	404	Total	C	N	O	P	S	0	0	0
			3280	2080	581	596	3	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	978	GLY	-	expression tag	UNP O75460
A	979	ASN	-	expression tag	UNP O75460
A	980	SER	-	expression tag	UNP O75460
B	978	GLY	-	expression tag	UNP O75460
B	979	ASN	-	expression tag	UNP O75460
B	980	SER	-	expression tag	UNP O75460
C	978	GLY	-	expression tag	UNP O75460
C	979	ASN	-	expression tag	UNP O75460
C	980	SER	-	expression tag	UNP O75460
D	978	GLY	-	expression tag	UNP O75460
D	979	ASN	-	expression tag	UNP O75460
D	980	SER	-	expression tag	UNP O75460

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	110	Total	O	0	0
			110	110		

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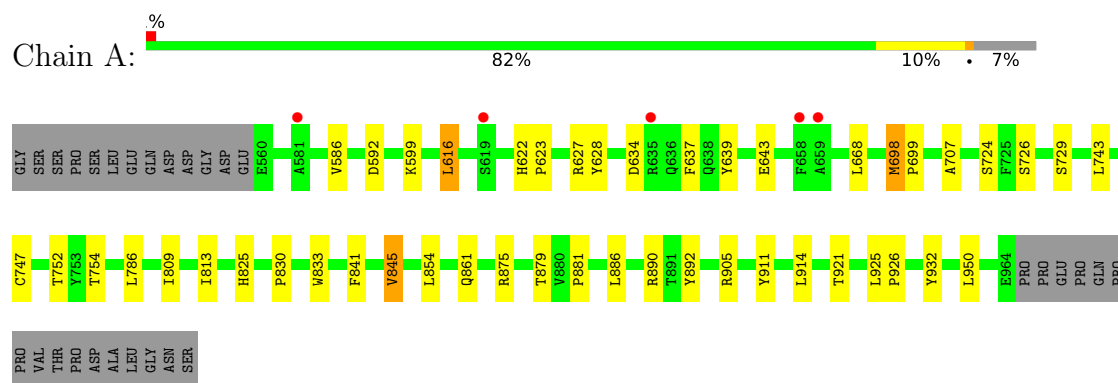
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	80	Total	O	0	0
			80	80		
2	D	85	Total	O	0	0
			85	85		

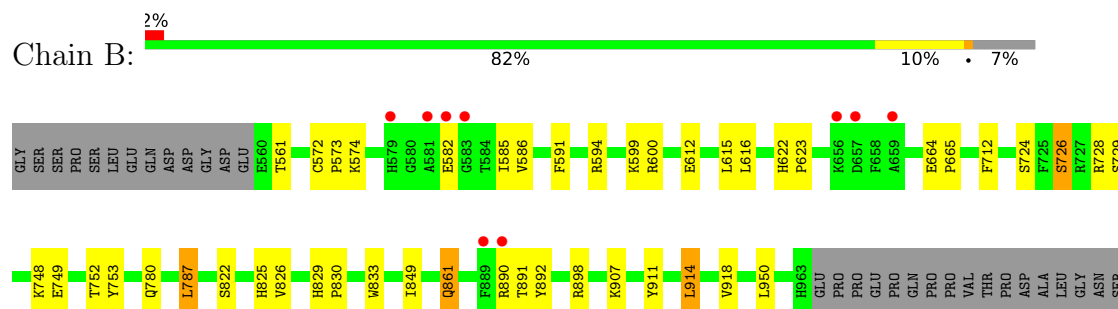
3 Residue-property plots [i](#)

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.

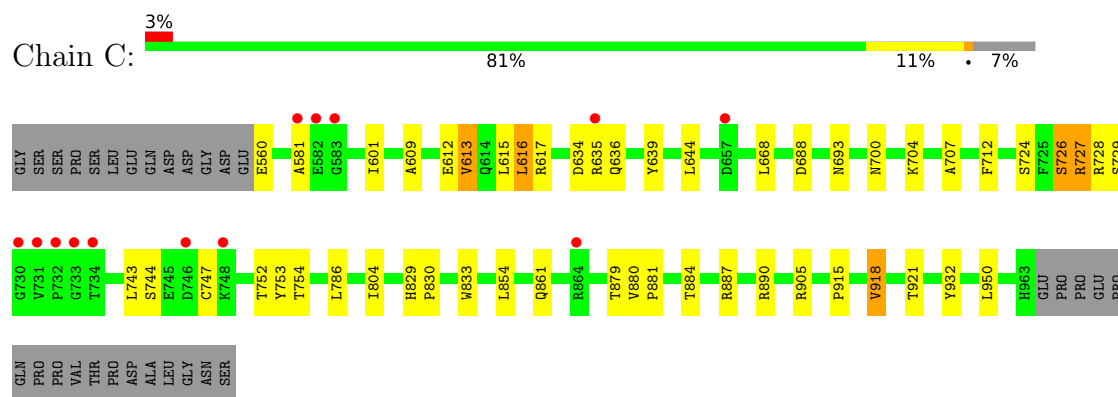
- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



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- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

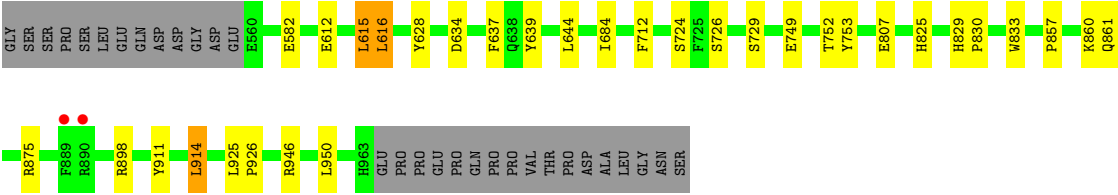


- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain D:

85%

7% • 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.49Å 158.66Å 155.94Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	47.48 – 2.30 47.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.48-2.30) 99.5 (47.48-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.248 0.209 , 0.250	Depositor DCC
R_{free} test set	4927 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for -h,-l,-k 0.030 for -h,l,k 0.080 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13478	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: 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	0.23	0/3332	0.39	0/4493
1	B	0.23	0/3327	0.39	0/4486
1	C	0.23	0/3327	0.39	0/4486
1	D	0.23	0/3327	0.39	0/4486
All	All	0.23	0/13313	0.39	0/17951

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 [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	3285	0	3245	24	0
1	B	3280	0	3243	24	0
1	C	3280	0	3242	30	0
1	D	3280	0	3243	16	0
2	A	78	0	0	0	0
2	B	110	0	0	2	0
2	C	80	0	0	0	0
2	D	85	0	0	3	0
All	All	13478	0	12973	91	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 (91) 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:890:ARG:O	1:B:892:TYR:N	2.25	0.69
1:A:592:ASP:O	1:C:617:ARG:NH1	2.26	0.69
1:A:861:GLN:HG3	1:A:950:LEU:HD11	1.74	0.68
1:B:849:ILE:O	1:B:898:ARG:NH1	2.27	0.67
1:C:688:ASP:O	1:C:693:ASN:ND2	2.29	0.65
1:A:875:ARG:NH2	1:A:886:LEU:O	2.33	0.62
1:B:574:LYS:NZ	2:B:1003:HOH:O	2.32	0.62
1:C:612:GLU:HG3	1:C:712:PHE:HB2	1.83	0.59
1:D:634:ASP:HB3	1:D:637:PHE:H	1.69	0.58
1:D:861:GLN:HG3	1:D:950:LEU:HD11	1.85	0.58
1:C:861:GLN:HG3	1:C:950:LEU:HD11	1.85	0.58
1:A:911:TYR:HA	1:A:914:LEU:HD22	1.86	0.56
1:B:664:GLU:HG3	1:B:665:PRO:HD2	1.89	0.55
1:D:857:PRO:HA	1:D:860:LYS:HE2	1.89	0.55
1:D:752:THR:OG1	1:D:753:TYR:N	2.39	0.54
1:D:634:ASP:HB2	1:D:639:TYR:HE1	1.72	0.54
1:C:726:SEP:O2P	1:C:728:ARG:NH1	2.40	0.54
1:C:879:THR:HG21	1:C:921:THR:HB	1.90	0.54
1:A:890:ARG:NH2	1:B:582:GLU:OE1	2.39	0.54
1:B:748:LYS:HG3	1:B:749:GLU:HG2	1.90	0.53
1:D:946:ARG:NH2	2:D:1001:HOH:O	2.31	0.52
1:B:591:PHE:O	1:B:594:ARG:HG2	2.10	0.52
1:B:612:GLU:HG3	1:B:712:PHE:HB2	1.92	0.52
1:D:911:TYR:HA	1:D:914:LEU:HD22	1.91	0.52
1:D:616:LEU:HG	1:D:628:TYR:HB2	1.92	0.51
1:A:830:PRO:HA	1:A:833:TRP:CG	2.46	0.51
1:C:879:THR:HG23	1:C:881:PRO:HD2	1.92	0.50
1:A:586:VAL:HG22	1:A:599:LYS:HG2	1.92	0.50
1:C:634:ASP:HB2	1:C:639:TYR:HE2	1.76	0.50
1:A:634:ASP:HB3	1:A:637:PHE:H	1.76	0.50
1:A:841:PHE:O	1:A:845:VAL:HG13	2.12	0.50
1:B:726:SEP:O1P	1:B:728:ARG:NH2	2.45	0.50
1:A:592:ASP:CG	1:C:617:ARG:HH12	2.15	0.50
1:B:752:THR:OG1	1:B:753:TYR:N	2.44	0.49
1:C:752:THR:OG1	1:C:753:TYR:N	2.43	0.49
1:C:879:THR:HG22	1:C:932:TYR:OH	2.12	0.49
1:C:880:VAL:HG22	1:C:881:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:VAL:O	1:C:617:ARG:HG3	2.14	0.47
1:D:830:PRO:HA	1:D:833:TRP:CG	2.49	0.47
1:A:875:ARG:NH1	1:A:892:TYR:O	2.46	0.47
1:A:743:LEU:HB2	1:A:786:LEU:HD21	1.96	0.47
1:B:861:GLN:HG3	1:B:950:LEU:HD11	1.96	0.46
1:C:884:THR:O	1:C:887:ARG:HG2	2.13	0.46
1:C:635:ARG:HG3	1:C:636:GLN:HG3	1.98	0.46
1:C:601:ILE:HG21	1:C:609:ALA:HB2	1.98	0.46
1:C:668:LEU:HG	1:C:707:ALA:HB2	1.98	0.45
1:C:727:ARG:HH22	1:C:747:CYS:HB3	1.81	0.45
1:C:915:PRO:HB2	1:C:918:VAL:HG13	1.99	0.45
1:A:881:PRO:HG2	1:A:921:THR:HG21	1.99	0.45
1:D:582:GLU:N	2:D:1011:HOH:O	2.50	0.45
1:C:743:LEU:HB2	1:C:786:LEU:HD21	1.99	0.44
1:D:807:GLU:OE2	1:D:829:HIS:NE2	2.29	0.44
1:C:830:PRO:HA	1:C:833:TRP:CG	2.52	0.44
1:C:881:PRO:HG2	1:C:921:THR:HG21	1.99	0.44
1:A:634:ASP:HB2	1:A:639:TYR:HE1	1.82	0.44
1:D:898:ARG:NE	2:D:1012:HOH:O	2.50	0.44
1:A:809:ILE:O	1:A:813:ILE:HG12	2.17	0.44
1:C:887:ARG:HB2	1:C:890:ARG:NH2	2.33	0.44
1:C:616:LEU:HA	1:C:616:LEU:HD12	1.90	0.44
1:C:829:HIS:CG	1:C:830:PRO:HD2	2.53	0.43
1:C:752:THR:HG23	1:C:754:THR:H	1.83	0.43
1:B:911:TYR:HA	1:B:914:LEU:HD22	2.00	0.43
1:A:925:LEU:HA	1:A:926:PRO:HA	1.81	0.43
1:B:574:LYS:HE3	1:B:574:LYS:HB2	1.80	0.43
1:B:586:VAL:HG22	1:B:599:LYS:HG2	2.01	0.43
1:D:612:GLU:HG3	1:D:712:PHE:HB2	2.00	0.43
1:B:622:HIS:CG	1:B:623:PRO:HD2	2.54	0.42
1:B:907:LYS:HA	1:B:907:LYS:HD3	1.81	0.42
1:A:627:ARG:HB3	1:A:643:GLU:HB2	2.01	0.42
1:A:668:LEU:HG	1:A:707:ALA:HB2	2.01	0.42
1:A:698:MET:HG3	1:A:699:PRO:HD2	2.01	0.42
1:A:616:LEU:HG	1:A:628:TYR:HB2	2.00	0.42
1:B:787:LEU:HA	1:B:787:LEU:HD12	1.90	0.42
1:B:829:HIS:CG	1:B:830:PRO:HD2	2.55	0.42
1:D:925:LEU:HA	1:D:926:PRO:HA	1.81	0.41
1:A:622:HIS:CG	1:A:623:PRO:HD2	2.56	0.41
1:A:879:THR:HG21	1:A:921:THR:HB	2.02	0.41
1:B:780:GLN:NE2	2:B:1017:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:SER:O	1:B:826:VAL:HG23	2.20	0.41
1:B:830:PRO:HA	1:B:833:TRP:CG	2.55	0.41
1:D:616:LEU:HD13	1:D:712:PHE:CD2	2.56	0.41
1:B:572:CYS:HA	1:B:573:PRO:HD3	1.95	0.41
1:C:879:THR:HG21	1:C:921:THR:CB	2.51	0.41
1:B:830:PRO:HA	1:B:833:TRP:CD2	2.55	0.41
1:D:615:LEU:HG	1:D:684:ILE:HD13	2.03	0.41
1:C:700:ASN:HD21	1:C:704:LYS:HB2	1.84	0.40
1:A:752:THR:HG23	1:A:754:THR:H	1.86	0.40
1:C:744:SER:HB3	1:C:747:CYS:HB2	2.03	0.40
1:A:879:THR:HG22	1:A:932:TYR:OH	2.20	0.40
1:B:585:ILE:HD12	1:B:600:ARG:NH2	2.36	0.40
1:C:830:PRO:HA	1:C:833:TRP:CD2	2.56	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	400/434 (92%)	385 (96%)	14 (4%)	1 (0%)	41	50
1	B	399/434 (92%)	386 (97%)	12 (3%)	1 (0%)	41	50
1	C	399/434 (92%)	382 (96%)	16 (4%)	1 (0%)	41	50
1	D	399/434 (92%)	384 (96%)	15 (4%)	0	100	100
All	All	1597/1736 (92%)	1537 (96%)	57 (4%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	891	THR
1	C	581	ALA

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Mol	Chain	Res	Type
1	A	747	CYS

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	355/381 (93%)	349 (98%)	6 (2%)	60	76
1	B	355/381 (93%)	347 (98%)	8 (2%)	50	67
1	C	355/381 (93%)	345 (97%)	10 (3%)	43	60
1	D	355/381 (93%)	348 (98%)	7 (2%)	55	72
All	All	1420/1524 (93%)	1389 (98%)	31 (2%)	52	69

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	616	LEU
1	A	698	MET
1	A	825	HIS
1	A	845	VAL
1	A	854	LEU
1	A	905	ARG
1	B	561	THR
1	B	615	LEU
1	B	616	LEU
1	B	787	LEU
1	B	825	HIS
1	B	861	GLN
1	B	914	LEU
1	B	918	VAL
1	C	560	GLU
1	C	613	VAL
1	C	615	LEU
1	C	616	LEU
1	C	644	LEU
1	C	727	ARG

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Mol	Chain	Res	Type
1	C	804	ILE
1	C	854	LEU
1	C	905	ARG
1	C	918	VAL
1	D	615	LEU
1	D	616	LEU
1	D	644	LEU
1	D	749	GLU
1	D	825	HIS
1	D	875	ARG
1	D	914	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	729	1	8,9,10	1.53	1 (12%)	8,12,14	1.51	2 (25%)
1	SEP	C	724	1	8,9,10	1.56	1 (12%)	8,12,14	1.32	2 (25%)
1	SEP	A	724	1	8,9,10	1.54	1 (12%)	8,12,14	1.47	2 (25%)
1	SEP	C	729	1	8,9,10	1.56	1 (12%)	8,12,14	1.75	2 (25%)
1	SEP	B	729	1	8,9,10	1.55	1 (12%)	8,12,14	1.29	2 (25%)
1	SEP	D	724	1	8,9,10	1.54	1 (12%)	8,12,14	1.32	2 (25%)
1	SEP	D	729	1	8,9,10	1.55	1 (12%)	8,12,14	1.33	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	B	724	1	8,9,10	1.54	1 (12%)	8,12,14	1.42	2 (25%)
1	SEP	A	726	1	8,9,10	1.53	1 (12%)	8,12,14	1.62	2 (25%)
1	SEP	B	726	1	8,9,10	1.55	1 (12%)	8,12,14	1.67	2 (25%)
1	SEP	C	726	1	8,9,10	1.55	1 (12%)	8,12,14	1.68	2 (25%)
1	SEP	D	726	1	8,9,10	1.55	1 (12%)	8,12,14	1.61	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	729	1	-	0/5/8/10	-
1	SEP	C	724	1	-	4/5/8/10	-
1	SEP	A	724	1	-	4/5/8/10	-
1	SEP	C	729	1	-	2/5/8/10	-
1	SEP	B	729	1	-	0/5/8/10	-
1	SEP	D	724	1	-	4/5/8/10	-
1	SEP	D	729	1	-	0/5/8/10	-
1	SEP	B	724	1	-	2/5/8/10	-
1	SEP	A	726	1	-	0/5/8/10	-
1	SEP	B	726	1	-	1/5/8/10	-
1	SEP	C	726	1	-	1/5/8/10	-
1	SEP	D	726	1	-	0/5/8/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	724	SEP	P-O1P	3.41	1.61	1.50
1	C	729	SEP	P-O1P	3.39	1.61	1.50
1	B	726	SEP	P-O1P	3.38	1.61	1.50
1	A	724	SEP	P-O1P	3.37	1.61	1.50
1	D	724	SEP	P-O1P	3.37	1.61	1.50
1	D	729	SEP	P-O1P	3.37	1.61	1.50
1	C	726	SEP	P-O1P	3.36	1.61	1.50
1	D	726	SEP	P-O1P	3.36	1.61	1.50
1	B	729	SEP	P-O1P	3.34	1.61	1.50
1	B	724	SEP	P-O1P	3.31	1.61	1.50
1	A	726	SEP	P-O1P	3.31	1.61	1.50
1	A	729	SEP	P-O1P	3.30	1.61	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	SEP	P-OG-CB	-3.43	108.86	118.30
1	B	726	SEP	P-OG-CB	-3.25	109.34	118.30
1	C	729	SEP	OG-CB-CA	3.23	111.29	108.14
1	C	729	SEP	P-OG-CB	-3.19	109.51	118.30
1	C	726	SEP	P-OG-CB	-3.17	109.56	118.30
1	C	726	SEP	OG-CB-CA	3.02	111.08	108.14
1	D	726	SEP	OG-CB-CA	3.00	111.06	108.14
1	B	726	SEP	OG-CB-CA	2.92	110.98	108.14
1	D	726	SEP	P-OG-CB	-2.88	110.36	118.30
1	A	724	SEP	OG-CB-CA	2.78	110.86	108.14
1	A	729	SEP	OG-CB-CA	2.70	110.77	108.14
1	A	729	SEP	P-OG-CB	-2.66	110.96	118.30
1	B	724	SEP	OG-CB-CA	2.63	110.71	108.14
1	A	726	SEP	OG-CB-CA	2.53	110.61	108.14
1	A	724	SEP	P-OG-CB	-2.49	111.44	118.30
1	D	724	SEP	P-OG-CB	-2.41	111.66	118.30
1	C	724	SEP	P-OG-CB	-2.41	111.67	118.30
1	B	724	SEP	P-OG-CB	-2.34	111.84	118.30
1	D	729	SEP	P-OG-CB	-2.32	111.90	118.30
1	D	729	SEP	OG-CB-CA	2.29	110.38	108.14
1	B	729	SEP	P-OG-CB	-2.26	112.08	118.30
1	B	729	SEP	OG-CB-CA	2.21	110.30	108.14
1	D	724	SEP	OG-CB-CA	2.17	110.25	108.14
1	C	724	SEP	OG-CB-CA	2.15	110.24	108.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	724	SEP	CB-OG-P-O2P
1	C	724	SEP	CB-OG-P-O3P
1	A	724	SEP	N-CA-CB-OG
1	A	724	SEP	CB-OG-P-O1P
1	A	724	SEP	CB-OG-P-O2P
1	A	724	SEP	CB-OG-P-O3P
1	C	729	SEP	N-CA-CB-OG
1	C	729	SEP	CB-OG-P-O2P
1	D	724	SEP	N-CA-CB-OG
1	D	724	SEP	CB-OG-P-O2P
1	D	724	SEP	CB-OG-P-O3P
1	B	724	SEP	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	B	726	SEP	N-CA-CB-OG
1	C	724	SEP	CB-OG-P-O1P
1	D	724	SEP	CB-OG-P-O1P
1	C	724	SEP	N-CA-CB-OG
1	C	726	SEP	CB-OG-P-O1P
1	B	724	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	726	SEP	1	0
1	C	726	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 [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	402/434 (92%)	-0.14	5 (1%) 79 83	33, 49, 81, 109	0
1	B	401/434 (92%)	-0.17	9 (2%) 62 69	33, 48, 77, 137	0
1	C	401/434 (92%)	-0.10	13 (3%) 47 54	35, 51, 93, 176	0
1	D	401/434 (92%)	-0.23	2 (0%) 91 94	33, 48, 76, 134	0
All	All	1605/1736 (92%)	-0.16	29 (1%) 68 74	33, 49, 81, 176	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	583	GLY	8.4
1	B	581	ALA	5.4
1	C	731	VAL	5.2
1	B	889	PHE	4.7
1	C	582	GLU	4.6
1	C	746	ASP	4.4
1	C	657	ASP	4.4
1	B	890	ARG	4.3
1	B	657	ASP	4.0
1	A	658	PHE	3.9
1	B	656	LYS	3.2
1	B	659	ALA	3.0
1	D	890	ARG	3.0
1	C	732	PRO	2.9
1	C	730	GLY	2.8
1	A	635	ARG	2.6
1	A	659	ALA	2.6
1	C	864	ARG	2.6
1	C	635	ARG	2.5
1	A	581	ALA	2.5
1	B	582	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	748	LYS	2.4
1	B	579	HIS	2.4
1	A	619	SER	2.4
1	B	583	GLY	2.3
1	C	733	GLY	2.3
1	D	889	PHE	2.2
1	C	734	THR	2.2
1	C	581	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	C	729	10/11	0.89	0.12	63,135,137,179	0
1	SEP	A	726	10/11	0.91	0.11	51,62,100,111	0
1	SEP	C	726	10/11	0.91	0.10	66,72,102,179	0
1	SEP	B	726	10/11	0.93	0.12	50,64,104,122	0
1	SEP	D	726	10/11	0.94	0.09	45,51,87,89	0
1	SEP	B	724	10/11	0.95	0.10	48,56,70,95	0
1	SEP	A	729	10/11	0.96	0.11	48,54,64,82	0
1	SEP	D	724	10/11	0.97	0.14	42,49,72,76	0
1	SEP	C	724	10/11	0.97	0.10	59,65,72,79	0
1	SEP	B	729	10/11	0.97	0.08	49,53,56,62	0
1	SEP	A	724	10/11	0.98	0.11	43,57,81,99	0
1	SEP	D	729	10/11	0.99	0.11	40,45,48,56	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 ⓘ

There are no such residues in this entry.