



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:47 AM UTC

PDB ID : 6W3C / pdb_00006w3c
Title : Structure of phosphorylated apo IRE1
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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 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

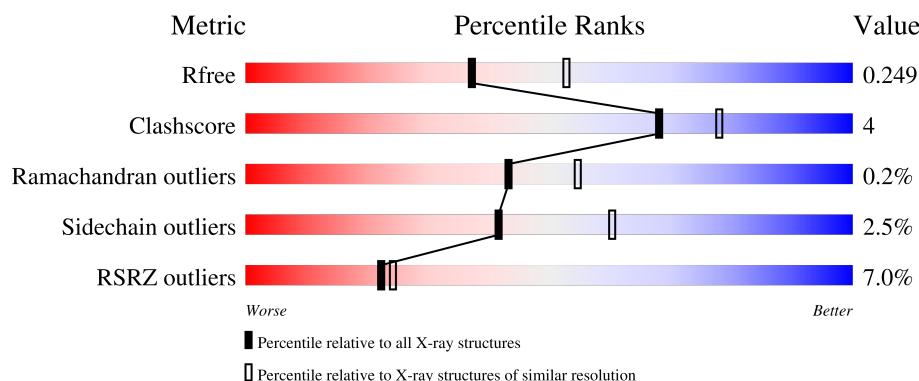
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	434	
1	B	434	
1	C	434	
1	D	434	

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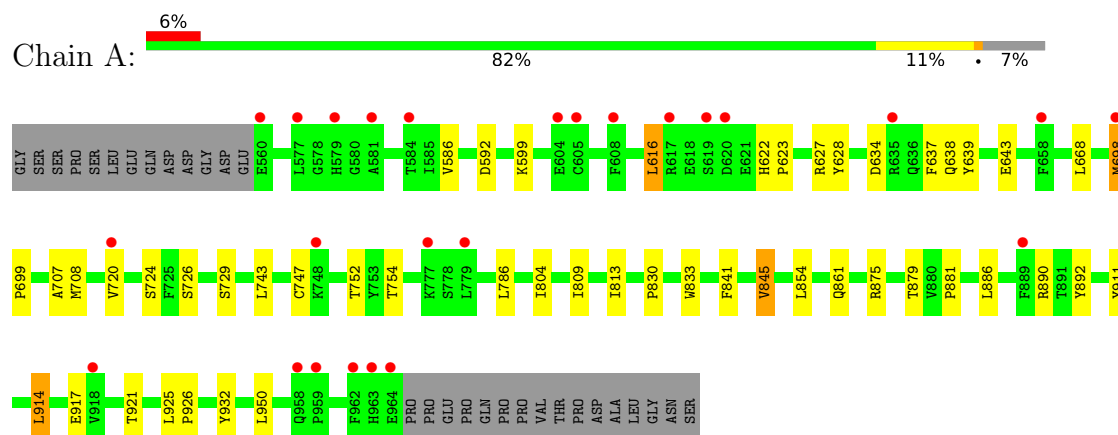
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	80	Total	O	0	0
			80	80		
2	D	85	Total	O	0	0
			85	85		

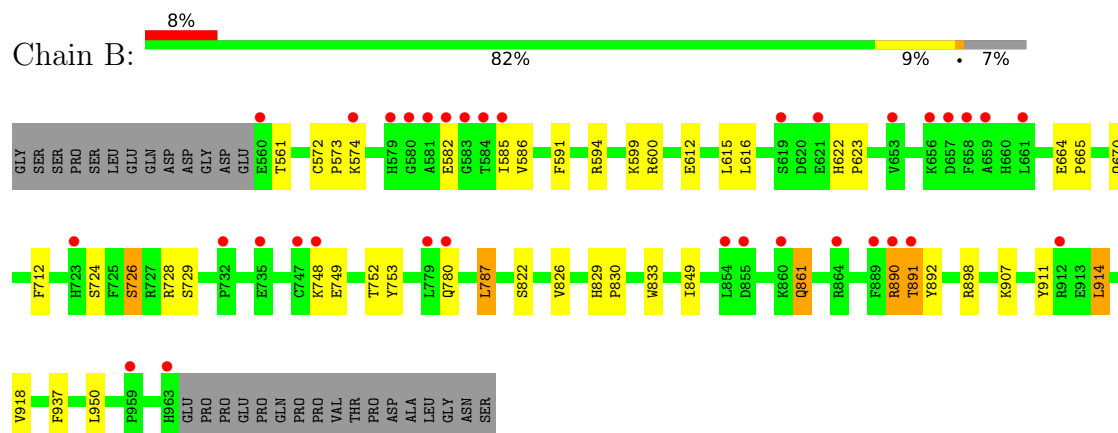
3 Residue-property plots

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.

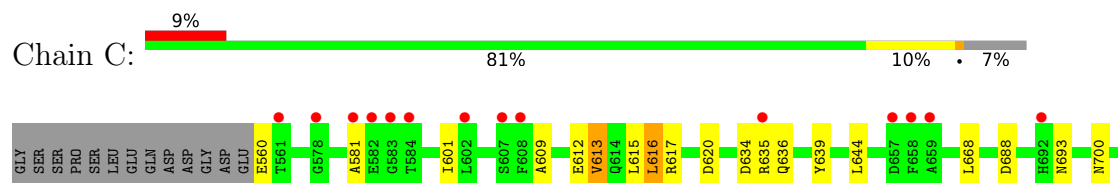
- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

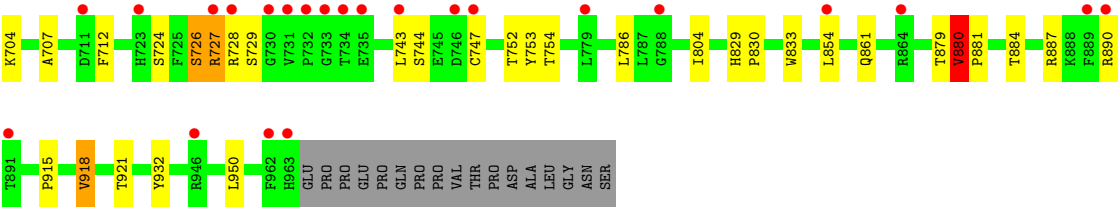


- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

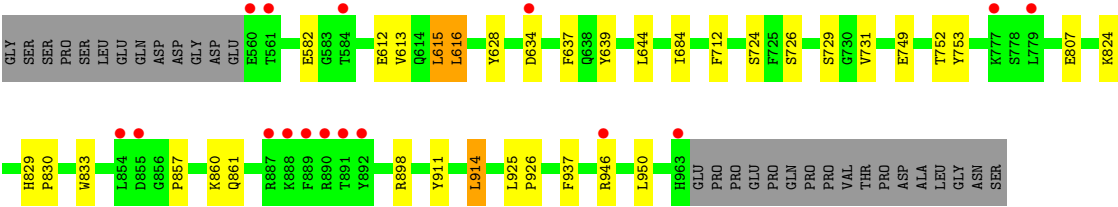
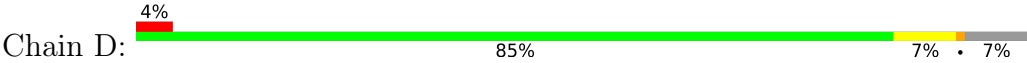


- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1





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



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 0.211 , 0.249	Depositor DCC
R_{free} test set	4927 reflections (4.82%)	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)	0.31 , 29.0	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	0.29	0/3332	0.71	0/4493
1	B	0.29	0/3327	0.70	2/4486 (0.0%)
1	C	0.28	0/3327	0.72	2/4486 (0.0%)
1	D	0.28	0/3327	0.70	2/4486 (0.0%)
All	All	0.28	0/13313	0.71	6/17951 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	937	PHE	CA-C-N	5.68	126.05	119.47
1	B	937	PHE	C-N-CA	5.68	126.05	119.47
1	D	937	PHE	CA-C-N	5.56	125.23	119.56
1	D	937	PHE	C-N-CA	5.56	125.23	119.56
1	C	880	VAL	CA-C-N	-5.53	113.33	119.19
1	C	880	VAL	C-N-CA	-5.53	113.33	119.19

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	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3280	0	3243	25	0
1	C	3280	0	3242	31	0
1	D	3280	0	3243	17	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	4	0
All	All	13478	0	12973	95	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 4.

All (95) 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	0.61
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:A:592:ASP:CG	1:C:617:ARG:HH12	2.15	0.55
1:D:857:PRO:HA	1:D:860:LYS:HE2	1.89	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:890:ARG:C	1:B:892:TYR:H	2.19	0.45
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:HD12	1:C:616:LEU:HA	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:D:752:THR:OG1	1:D:753:TYR:N	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:HIS:CG	1:B:623:PRO:HD2	2.54	0.42
1:A:627:ARG:HH22	1:C:620:ASP:CG	2.26	0.42
1:B:907:LYS:HD3	1:B:907:LYS:HA	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:HD12	1:B:787:LEU:HA	1.90	0.42
1:B:829:HIS:CG	1:B:830:PRO:HD2	2.55	0.42
1:A:708:MET:HE3	1:A:708:MET:HB2	1.94	0.42
1:D:824:LYS:NZ	2:D:1016:HOH:O	2.52	0.41
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
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%)	36	46
1	B	399/434 (92%)	386 (97%)	12 (3%)	1 (0%)	36	46
1	C	399/434 (92%)	382 (96%)	16 (4%)	1 (0%)	36	46
1	D	399/434 (92%)	384 (96%)	15 (4%)	0	100	100
All	All	1597/1736 (92%)	1537 (96%)	57 (4%)	3 (0%)	43	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	891	THR
1	C	581	ALA
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%)	346 (98%)	9 (2%)	42	60
1	B	355/381 (93%)	345 (97%)	10 (3%)	38	56
1	C	355/381 (93%)	345 (97%)	10 (3%)	38	56
1	D	355/381 (93%)	348 (98%)	7 (2%)	48	67
All	All	1420/1524 (93%)	1384 (98%)	36 (2%)	42	60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	616	LEU
1	A	638	GLN
1	A	698	MET
1	A	720	VAL
1	A	804	ILE
1	A	845	VAL
1	A	854	LEU
1	A	914	LEU

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Mol	Chain	Res	Type
1	A	917	GLU
1	B	561	THR
1	B	615	LEU
1	B	616	LEU
1	B	670	GLN
1	B	787	LEU
1	B	861	GLN
1	B	890	ARG
1	B	891	THR
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
1	C	804	ILE
1	C	854	LEU
1	C	880	VAL
1	C	918	VAL
1	D	613	VAL
1	D	615	LEU
1	D	616	LEU
1	D	644	LEU
1	D	731	VAL
1	D	749	GLU
1	D	914	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	660	HIS
1	A	683	ASN
1	A	723	HIS
1	A	939	HIS
1	B	678	HIS
1	B	796	HIS
1	B	800	HIS
1	C	614	GLN
1	C	683	ASN
1	C	800	HIS

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Mol	Chain	Res	Type
1	C	906	ASN
1	D	614	GLN
1	D	683	ASN
1	D	723	HIS
1	D	909	HIS
1	D	939	HIS

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	D	724	1	8,9,10	1.61	1 (12%)	7,12,14	1.10	1 (14%)
1	SEP	A	726	1	8,9,10	1.59	1 (12%)	7,12,14	1.16	1 (14%)
1	SEP	B	724	1	8,9,10	1.60	1 (12%)	7,12,14	1.25	1 (14%)
1	SEP	C	726	1	8,9,10	1.62	1 (12%)	7,12,14	1.35	1 (14%)
1	SEP	A	724	1	8,9,10	1.61	1 (12%)	7,12,14	1.28	1 (14%)
1	SEP	B	726	1	8,9,10	1.61	1 (12%)	7,12,14	1.32	1 (14%)
1	SEP	D	729	1	8,9,10	1.62	1 (12%)	7,12,14	1.13	1 (14%)
1	SEP	C	729	1	8,9,10	1.62	1 (12%)	7,12,14	1.45	1 (14%)
1	SEP	A	729	1	8,9,10	1.59	1 (12%)	7,12,14	1.27	1 (14%)
1	SEP	D	726	1	8,9,10	1.61	1 (12%)	7,12,14	1.34	1 (14%)
1	SEP	C	724	1	8,9,10	1.62	1 (12%)	7,12,14	1.10	1 (14%)
1	SEP	B	729	1	8,9,10	1.61	1 (12%)	7,12,14	1.10	1 (14%)

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	D	724	1	-	5/6/8/10	-
1	SEP	A	726	1	-	0/6/8/10	-
1	SEP	B	724	1	-	3/6/8/10	-
1	SEP	C	726	1	-	1/6/8/10	-
1	SEP	A	724	1	-	5/6/8/10	-
1	SEP	B	726	1	-	2/6/8/10	-
1	SEP	D	729	1	-	0/6/8/10	-
1	SEP	C	729	1	-	3/6/8/10	-
1	SEP	A	729	1	-	0/6/8/10	-
1	SEP	D	726	1	-	0/6/8/10	-
1	SEP	C	724	1	-	5/6/8/10	-
1	SEP	B	729	1	-	0/6/8/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	724	SEP	P-O1P	3.56	1.61	1.50
1	C	729	SEP	P-O1P	3.53	1.61	1.50
1	B	726	SEP	P-O1P	3.53	1.61	1.50
1	A	724	SEP	P-O1P	3.52	1.61	1.50
1	D	724	SEP	P-O1P	3.52	1.61	1.50
1	D	729	SEP	P-O1P	3.51	1.61	1.50
1	C	726	SEP	P-O1P	3.51	1.61	1.50
1	D	726	SEP	P-O1P	3.50	1.61	1.50
1	B	729	SEP	P-O1P	3.49	1.61	1.50
1	B	724	SEP	P-O1P	3.46	1.61	1.50
1	A	726	SEP	P-O1P	3.45	1.61	1.50
1	A	729	SEP	P-O1P	3.45	1.61	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	729	SEP	OG-CB-CA	3.23	111.29	108.14
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	D	729	SEP	OG-CB-CA	2.29	110.38	108.14
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 (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	724	SEP	N-CA-CB-OG
1	A	724	SEP	C-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	B	724	SEP	N-CA-CB-OG
1	B	724	SEP	C-CA-CB-OG
1	B	726	SEP	N-CA-CB-OG
1	B	726	SEP	C-CA-CB-OG
1	C	724	SEP	C-CA-CB-OG
1	C	724	SEP	CB-OG-P-O2P
1	C	724	SEP	CB-OG-P-O3P
1	C	729	SEP	N-CA-CB-OG
1	C	729	SEP	C-CA-CB-OG
1	C	729	SEP	CB-OG-P-O2P
1	D	724	SEP	N-CA-CB-OG
1	D	724	SEP	C-CA-CB-OG
1	D	724	SEP	CB-OG-P-O2P
1	D	724	SEP	CB-OG-P-O3P
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	C	726	SEP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	726	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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%)	0.62	25 (6%)	26	28	33, 49, 81, 109	0
1	B	401/434 (92%)	0.52	34 (8%)	16	18	33, 48, 77, 137	0
1	C	401/434 (92%)	0.63	37 (9%)	14	16	35, 51, 93, 176	0
1	D	401/434 (92%)	0.48	16 (3%)	42	44	33, 48, 76, 134	0
All	All	1605/1736 (92%)	0.56	112 (6%)	22	24	33, 49, 81, 176	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	731	VAL	8.2
1	C	732	PRO	6.2
1	B	581	ALA	5.7
1	C	583	GLY	5.7
1	D	891	THR	5.5
1	B	890	ARG	5.1
1	A	658	PHE	5.1
1	A	964	GLU	4.8
1	C	582	GLU	4.7
1	B	657	ASP	4.6
1	D	779	LEU	4.6
1	C	733	GLY	4.5
1	C	730	GLY	4.4
1	C	581	ALA	4.4
1	A	779	LEU	4.4
1	D	890	ARG	4.1
1	D	963	HIS	4.0
1	B	889	PHE	4.0
1	A	720	VAL	3.8
1	C	963	HIS	3.8
1	D	888	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	963	HIS	3.8
1	C	854	LEU	3.7
1	D	889	PHE	3.6
1	A	619	SER	3.5
1	B	659	ALA	3.5
1	B	656	LYS	3.5
1	C	657	ASP	3.4
1	A	963	HIS	3.4
1	C	746	ASP	3.1
1	D	887	ARG	3.1
1	B	584	THR	3.0
1	C	779	LEU	3.0
1	B	583	GLY	3.0
1	D	855	ASP	2.9
1	B	579	HIS	2.9
1	D	561	THR	2.9
1	B	621	GLU	2.8
1	B	779	LEU	2.8
1	A	918	VAL	2.8
1	B	723	HIS	2.7
1	C	561	THR	2.7
1	B	580	GLY	2.7
1	A	577	LEU	2.7
1	B	912	ARG	2.7
1	B	780	GLN	2.7
1	C	692	HIS	2.7
1	A	608	PHE	2.7
1	C	635	ARG	2.7
1	B	732	PRO	2.7
1	D	946	ARG	2.7
1	A	635	ARG	2.6
1	C	734	THR	2.6
1	C	607	SER	2.6
1	B	582	GLU	2.5
1	D	560	GLU	2.5
1	C	723	HIS	2.5
1	A	605	CYS	2.5
1	C	864	ARG	2.5
1	A	698	MET	2.5
1	C	962	PHE	2.4
1	A	777	LYS	2.4
1	C	602	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	579	HIS	2.4
1	C	608	PHE	2.4
1	B	860	LYS	2.3
1	C	747	CYS	2.3
1	B	661	LEU	2.3
1	C	659	ALA	2.3
1	C	890	ARG	2.3
1	A	958	GLN	2.3
1	C	578	GLY	2.3
1	C	728	ARG	2.3
1	A	584	THR	2.3
1	D	584	THR	2.3
1	A	560	GLU	2.3
1	D	634	ASP	2.2
1	C	946	ARG	2.2
1	B	574	LYS	2.2
1	C	889	PHE	2.2
1	A	581	ALA	2.2
1	D	777	LYS	2.2
1	B	854	LEU	2.2
1	A	889	PHE	2.2
1	B	748	LYS	2.2
1	C	891	THR	2.2
1	C	735	GLU	2.2
1	C	788	GLY	2.2
1	A	959	PRO	2.1
1	B	959	PRO	2.1
1	D	892	TYR	2.1
1	A	748	LYS	2.1
1	B	653	VAL	2.1
1	A	962	PHE	2.1
1	B	735	GLU	2.1
1	C	743	LEU	2.1
1	B	855	ASP	2.1
1	A	617	ARG	2.1
1	B	891	THR	2.1
1	B	560	GLU	2.1
1	D	854	LEU	2.1
1	B	585	ILE	2.1
1	B	864	ARG	2.1
1	B	619	SER	2.0
1	B	747	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	658	PHE	2.0
1	C	658	PHE	2.0
1	A	604	GLU	2.0
1	C	584	THR	2.0
1	A	620	ASP	2.0
1	C	711	ASP	2.0
1	C	727	ARG	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	0.73	0.15	63,135,137,179	0
1	SEP	B	726	10/11	0.82	0.14	50,64,104,122	0
1	SEP	A	726	10/11	0.82	0.12	51,62,100,111	0
1	SEP	C	726	10/11	0.83	0.12	66,72,102,179	0
1	SEP	B	724	10/11	0.89	0.11	48,56,70,95	0
1	SEP	D	726	10/11	0.89	0.10	45,51,87,89	0
1	SEP	A	729	10/11	0.91	0.11	48,54,64,82	0
1	SEP	C	724	10/11	0.93	0.10	59,65,72,79	0
1	SEP	D	724	10/11	0.94	0.10	42,49,72,76	0
1	SEP	B	729	10/11	0.95	0.08	49,53,56,62	0
1	SEP	A	724	10/11	0.95	0.08	43,57,81,99	0
1	SEP	D	729	10/11	0.97	0.06	40,45,48,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.