



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:47 PM GMT

PDB ID : 4Z7H
Title : Crystal structure of human IRE1 cytoplasmic kinase-RNase region - complex with imidazopyridine compound 3
Authors : Joshi, A.; Bayliss, R.
Deposited on : 2015-04-07
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

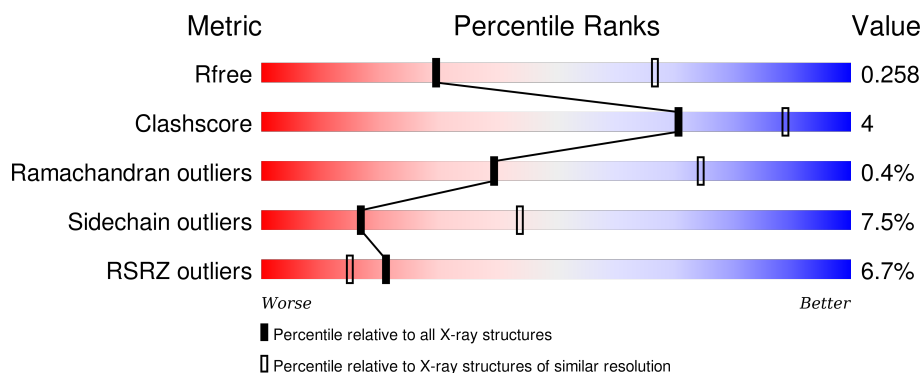
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	416	<div> <div>8%</div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div>
1	B	416	<div> <div>4%</div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div>

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
2	4L5	B	1001	-	-	-	X

2 Entry composition [i](#)

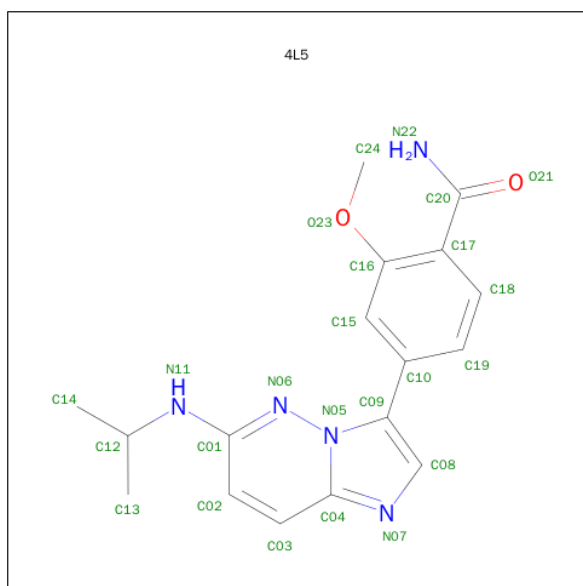
There are 4 unique types of molecules in this entry. The entry contains 6298 atoms, of which 38 are hydrogens and 0 are deuteriums.

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	385	Total	C	N	O	S	0	0	0
			3072	1962	536	555	19			
1	B	388	Total	C	N	O	S	0	0	0
			3114	1991	546	558	19			

- Molecule 2 is 2-methoxy-4-[6-(propan-2-ylamino)imidazo[1,2-b]pyridazin-3-yl]benzamide (three-letter code: 4L5) (formula: C₁₇H₁₉N₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			43	17	19	5	2		
2	B	1	Total	C	H	N	O	0	0
			43	17	19	5	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

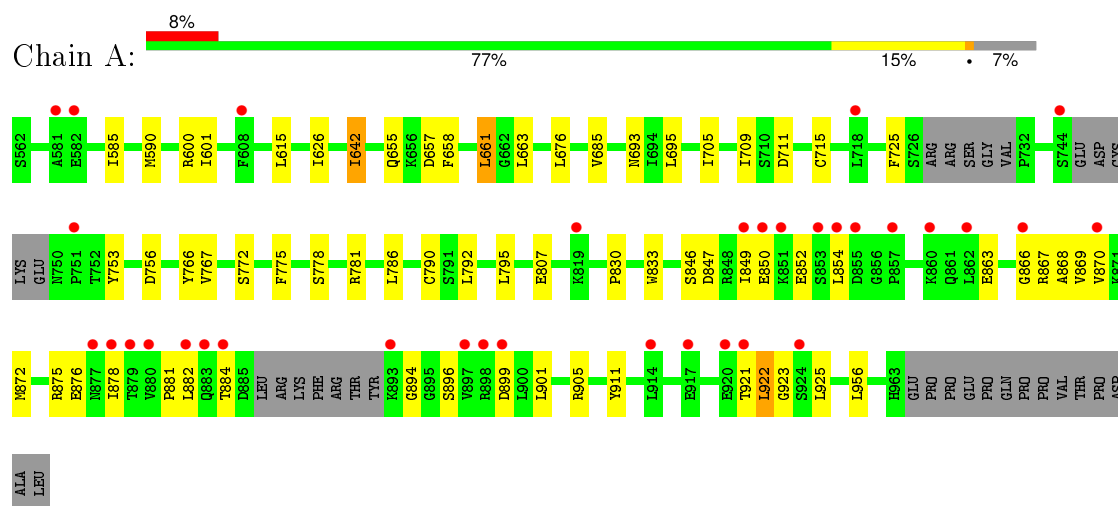
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	9	Total	O	0	0
			9	9		

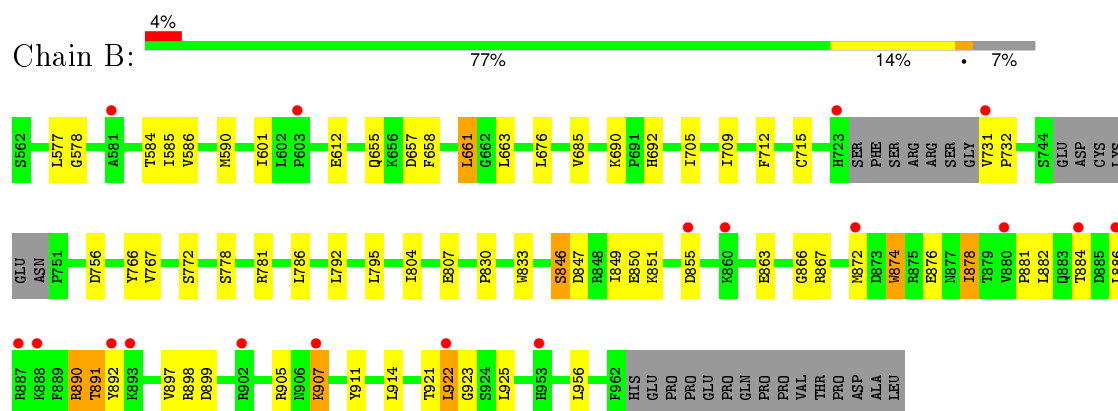
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.68Å 81.96Å 168.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 2.90 46.36 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.36-2.90) 99.6 (46.36-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.200 , 0.225 0.228 , 0.258	Depositor DCC
R_{free} test set	1260 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.6	EDS
Estimated twinning fraction	0.041 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 24771 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6298	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.84 % 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 2.0486e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, 4L5

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	0.48	0/3145	0.69	0/4247
1	B	0.50	0/3189	0.71	1/4307 (0.0%)
All	All	0.49	0/6334	0.70	1/8554 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	890	ARG	C-N-CA	5.13	134.52	121.70

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	3072	0	3026	26	0
1	B	3114	0	3086	26	0
2	A	24	19	19	1	0
2	B	24	19	19	3	0
3	A	5	0	0	0	0
4	A	12	0	0	0	0
4	B	9	0	0	0	0
All	All	6260	38	6150	55	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 (55) 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:584:THR:HG22	1:B:601:ILE:HA	1.72	0.72
1:B:577:LEU:HB2	1:B:586:VAL:HG23	1.76	0.67
1:B:658:PHE:O	1:B:661:LEU:HB2	1.95	0.66
1:A:658:PHE:O	1:A:661:LEU:HB2	1.97	0.65
1:A:881:PRO:HG2	1:A:921:THR:HG21	1.79	0.65
1:A:626:ILE:HD12	1:A:695:LEU:HD12	1.77	0.65
1:A:866:GLY:HA2	1:A:868:ALA:N	2.11	0.64
1:B:881:PRO:HG2	1:B:921:THR:HG21	1.79	0.63
1:B:712:PHE:HA	1:B:715:CYS:SG	2.39	0.63
1:A:850:GLU:H	1:A:852:GLU:HB2	1.66	0.60
1:B:907:LYS:HE2	1:B:914:LEU:HD13	1.85	0.57
1:B:921:THR:HG23	1:B:922:LEU:HD12	1.88	0.56
1:A:921:THR:HG23	1:A:922:LEU:HD12	1.89	0.55
1:A:693:ASN:ND2	1:A:711:ASP:HB2	2.24	0.53
1:A:866:GLY:HA2	1:A:868:ALA:H	1.75	0.52
1:B:690:LYS:HE2	1:B:692:HIS:HB3	1.93	0.51
1:A:866:GLY:HA3	1:A:869:VAL:H	1.75	0.51
1:A:626:ILE:HG23	1:A:642:ILE:HD11	1.92	0.50
1:A:911:TYR:OH	1:A:923:GLY:HA3	2.12	0.50
1:B:874:TRP:HD1	1:B:878:ILE:HD12	1.77	0.50
1:A:896:SER:HB3	1:A:899:ASP:HB2	1.93	0.50
1:B:911:TYR:OH	1:B:923:GLY:HA3	2.12	0.49
1:B:612:GLU:HG3	1:B:712:PHE:HB2	1.93	0.49
2:B:1001:4L5:N06	2:B:1001:4L5:H132	2.29	0.48
1:A:846:SER:HA	1:A:849:ILE:HG13	1.95	0.48
1:A:875:ARG:HE	1:A:894:GLY:HA3	1.79	0.48
1:B:663:LEU:HD21	1:B:705:ILE:HB	1.96	0.47
1:B:685:VAL:O	1:B:715:CYS:HA	2.15	0.47
1:A:663:LEU:HD21	1:A:705:ILE:HB	1.97	0.47
1:B:792:LEU:HB3	1:B:795:LEU:HD12	1.97	0.47
1:B:731:VAL:N	1:B:732:PRO:HD3	2.30	0.46
1:B:850:GLU:HA	1:B:898:ARG:HH21	1.81	0.46
2:A:1001:4L5:N06	2:A:1001:4L5:H132	2.31	0.46
2:B:1001:4L5:H151	2:B:1001:4L5:H132	1.98	0.46
1:A:585:ILE:HD11	1:A:600:ARG:NH2	2.30	0.46
1:A:685:VAL:HG22	1:A:753:TYR:CD1	2.51	0.46
1:A:792:LEU:HB3	1:A:795:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:847:ASP:OD1	1:B:905:ARG:HD2	2.17	0.45
1:A:615:LEU:HD13	1:A:715:CYS:HB2	1.98	0.45
1:B:850:GLU:HA	1:B:851:LYS:HA	1.79	0.45
1:B:578:GLY:HA3	2:B:1001:4L5:H141	1.98	0.43
1:B:890:ARG:HA	1:B:891:THR:HG22	1.99	0.43
1:A:676:LEU:HD11	1:A:756:ASP:HB3	2.00	0.43
1:A:847:ASP:OD1	1:A:905:ARG:HD2	2.18	0.42
1:A:766:TYR:HA	1:A:772:SER:O	2.19	0.42
1:A:882:LEU:HD22	1:A:922:LEU:HD11	2.01	0.42
1:A:830:PRO:HA	1:A:833:TRP:CD2	2.54	0.42
1:A:775:PHE:CE2	1:A:790:CYS:HB3	2.54	0.42
1:B:846:SER:OG	1:B:905:ARG:HD3	2.20	0.42
1:B:766:TYR:HA	1:B:772:SER:O	2.20	0.42
1:B:676:LEU:HD11	1:B:756:ASP:HB3	2.01	0.41
1:B:830:PRO:HA	1:B:833:TRP:CD2	2.55	0.41
1:B:882:LEU:HD22	1:B:922:LEU:HD11	2.02	0.41
1:B:778:SER:HA	1:B:781:ARG:HD2	2.02	0.41
1:A:778:SER:HA	1:A:781:ARG:HD2	2.03	0.41

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	377/416 (91%)	346 (92%)	30 (8%)	1 (0%)	46	79
1	B	382/416 (92%)	349 (91%)	31 (8%)	2 (0%)	34	71
All	All	759/832 (91%)	695 (92%)	61 (8%)	3 (0%)	39	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	867	ARG
1	B	867	ARG
1	B	866	GLY

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	333/369 (90%)	311 (93%)	22 (7%)	21	51
1	B	338/369 (92%)	310 (92%)	28 (8%)	14	38
All	All	671/738 (91%)	621 (92%)	50 (8%)	17	44

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	590	MET
1	A	601	ILE
1	A	642	ILE
1	A	655	GLN
1	A	657	ASP
1	A	661	LEU
1	A	709	ILE
1	A	725	PHE
1	A	767	VAL
1	A	786	LEU
1	A	807	GLU
1	A	854	LEU
1	A	863	GLU
1	A	870	VAL
1	A	872	MET
1	A	876	GLU
1	A	878	ILE
1	A	884	THR
1	A	901	LEU
1	A	922	LEU
1	A	925	LEU

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Mol	Chain	Res	Type
1	A	956	LEU
1	B	585	ILE
1	B	590	MET
1	B	655	GLN
1	B	657	ASP
1	B	661	LEU
1	B	709	ILE
1	B	767	VAL
1	B	786	LEU
1	B	804	ILE
1	B	807	GLU
1	B	846	SER
1	B	849	ILE
1	B	855	ASP
1	B	863	GLU
1	B	872	MET
1	B	874	TRP
1	B	876	GLU
1	B	878	ILE
1	B	884	THR
1	B	886	LEU
1	B	891	THR
1	B	892	TYR
1	B	897	VAL
1	B	899	ASP
1	B	907	LYS
1	B	922	LEU
1	B	925	LEU
1	B	956	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	693	ASN
1	A	909	HIS
1	A	910	HIS
1	B	678	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	4L5	A	1001	-	22,26,26	2.24	8 (36%)	26,37,37	1.83	7 (26%)
3	SO4	A	1002	-	4,4,4	0.11	0	6,6,6	0.17	0
2	4L5	B	1001	-	22,26,26	2.22	8 (36%)	26,37,37	1.56	7 (26%)

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	4L5	A	1001	-	-	0/14/14/14	0/3/3/3
3	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	4L5	B	1001	-	-	0/14/14/14	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	4L5	C17-C20	2.32	1.52	1.50
2	A	1001	4L5	C17-C20	2.35	1.53	1.50
2	B	1001	4L5	C01-N11	2.60	1.41	1.36
2	B	1001	4L5	O23-C16	2.63	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	4L5	O23-C16	2.97	1.41	1.37
2	A	1001	4L5	C03-C04	3.11	1.45	1.40
2	B	1001	4L5	C10-C09	3.23	1.52	1.48
2	A	1001	4L5	C10-C09	3.26	1.52	1.48
2	A	1001	4L5	C01-N11	3.29	1.43	1.36
2	A	1001	4L5	C03-C02	3.48	1.44	1.36
2	B	1001	4L5	C03-C04	3.67	1.46	1.40
2	B	1001	4L5	C03-C02	3.73	1.44	1.36
2	B	1001	4L5	C20-N22	4.55	1.42	1.33
2	A	1001	4L5	C04-N07	4.58	1.37	1.33
2	B	1001	4L5	C04-N07	4.61	1.37	1.33
2	A	1001	4L5	C20-N22	4.80	1.42	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	4L5	C16-C17-C20	-3.63	121.81	125.03
2	B	1001	4L5	O21-C20-N22	-3.54	117.61	122.59
2	A	1001	4L5	O21-C20-N22	-3.54	117.62	122.59
2	A	1001	4L5	O23-C16-C15	-2.86	119.33	124.21
2	B	1001	4L5	O23-C16-C15	-2.61	119.76	124.21
2	B	1001	4L5	C03-C02-C01	-2.13	115.74	118.45
2	B	1001	4L5	C16-C17-C20	-2.08	123.18	125.03
2	B	1001	4L5	C17-C20-N22	2.58	121.89	118.12
2	B	1001	4L5	O23-C16-C17	2.62	119.77	116.54
2	A	1001	4L5	C17-C20-N22	2.77	122.18	118.12
2	A	1001	4L5	C13-C12-N11	2.93	115.30	109.67
2	A	1001	4L5	O23-C16-C17	3.15	120.42	116.54
2	B	1001	4L5	C10-C09-N05	3.19	128.43	123.48
2	A	1001	4L5	C10-C09-N05	3.54	128.98	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	4L5	1	0
2	B	1001	4L5	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	385/416 (92%)	0.56	34 (8%) 12 8	40, 79, 154, 179	0
1	B	388/416 (93%)	0.40	18 (4%) 36 30	41, 78, 138, 169	0
All	All	773/832 (92%)	0.48	52 (6%) 21 15	40, 79, 146, 179	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	855	ASP	6.5
1	B	731	VAL	6.3
1	B	581	ALA	6.1
1	A	581	ALA	5.7
1	A	884	THR	5.1
1	B	892	TYR	4.5
1	B	887	ARG	4.5
1	A	855	ASP	4.3
1	A	897	VAL	4.0
1	A	877	ASN	4.0
1	A	857	PRO	3.9
1	A	854	LEU	3.8
1	A	898	ARG	3.7
1	A	924	SER	3.7
1	B	603	PRO	3.6
1	B	880	VAL	3.4
1	A	880	VAL	3.3
1	B	886	LEU	3.2
1	A	893	LYS	3.2
1	A	850	GLU	3.2
1	B	893	LYS	3.1
1	A	582	GLU	2.9
1	A	849	ILE	2.9
1	B	860	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	882	LEU	2.7
1	A	862	LEU	2.7
1	A	899	ASP	2.7
1	B	884	THR	2.7
1	A	917	GLU	2.6
1	A	608	PHE	2.6
1	A	819	LYS	2.6
1	A	718	LEU	2.6
1	A	879	THR	2.5
1	A	853	SER	2.5
1	A	860	LYS	2.5
1	A	920	GLU	2.4
1	B	888	LYS	2.4
1	B	953	HIS	2.4
1	A	870	VAL	2.4
1	A	914	LEU	2.4
1	A	878	ILE	2.4
1	B	922	LEU	2.2
1	A	883	GLN	2.2
1	B	907	LYS	2.2
1	B	872	MET	2.2
1	A	866	GLY	2.1
1	A	921	THR	2.1
1	A	751	PRO	2.1
1	B	902	ARG	2.1
1	B	723	HIS	2.1
1	A	744	SER	2.0
1	A	851	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	4L5	B	1001	24/24	0.96	0.31	2.60	68,77,94,94	0
2	4L5	A	1001	24/24	0.97	0.26	0.78	55,61,69,70	0
3	SO4	A	1002	5/5	0.85	0.16	-	128,128,129,130	0

6.5 Other polymers

There are no such residues in this entry.