wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2023 – 07:44 PM JST

PDB ID	:	4YR8
Title	:	Crystal structure of JNK in complex with a regulator protein
Authors	:	Liu, X.; Wang, J.; Wu, J.W.; Wang, Z.X.
Deposited on	:	2015-03-14
Resolution	:	2.40 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 (i) 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 (1)) were used in the production of this report:

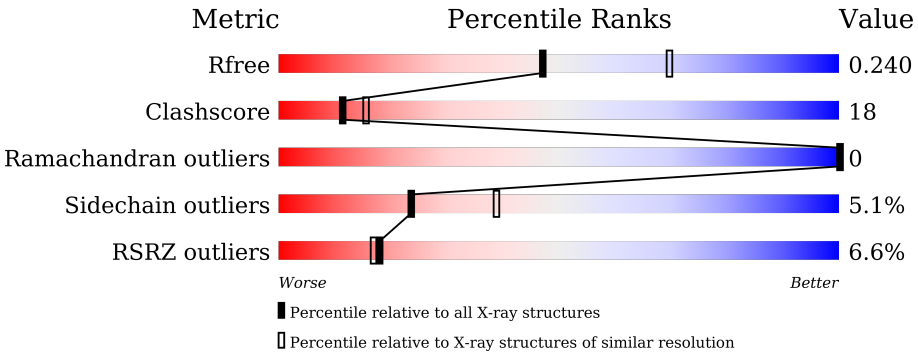
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	371	4% 67% 19% • 14%
1	C	371	10% 56% 27% • 14%
1	E	371	2% 58% 25% • 15%
1	F	371	9% 54% 24% • 19%
2	B	167	2% 68% 16% • 16%
2	D	167	4% 66% 19% 15%

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Mol	Chain	Length	Quality of chain
2	G	167	5% 56% 28% 16%
2	H	167	4% 66% 19% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14988 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 Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	317	Total	C	N	O	S	0	0	0
			2551	1639	430	463	19			
1	A	320	Total	C	N	O	S	0	0	0
			2582	1661	433	469	19			
1	C	318	Total	C	N	O	S	0	0	0
			2565	1652	431	463	19			
1	F	300	Total	C	N	O	S	0	1	0
			2412	1558	404	431	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	364	LEU	-	expression tag	UNP P45983
E	365	GLU	-	expression tag	UNP P45983
E	366	HIS	-	expression tag	UNP P45983
E	367	HIS	-	expression tag	UNP P45983
E	368	HIS	-	expression tag	UNP P45983
E	369	HIS	-	expression tag	UNP P45983
E	370	HIS	-	expression tag	UNP P45983
E	371	HIS	-	expression tag	UNP P45983
A	364	LEU	-	expression tag	UNP P45983
A	365	GLU	-	expression tag	UNP P45983
A	366	HIS	-	expression tag	UNP P45983
A	367	HIS	-	expression tag	UNP P45983
A	368	HIS	-	expression tag	UNP P45983
A	369	HIS	-	expression tag	UNP P45983
A	370	HIS	-	expression tag	UNP P45983
A	371	HIS	-	expression tag	UNP P45983
C	364	LEU	-	expression tag	UNP P45983
C	365	GLU	-	expression tag	UNP P45983
C	366	HIS	-	expression tag	UNP P45983
C	367	HIS	-	expression tag	UNP P45983
C	368	HIS	-	expression tag	UNP P45983

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Chain	Residue	Modelled	Actual	Comment	Reference
C	369	HIS	-	expression tag	UNP P45983
C	370	HIS	-	expression tag	UNP P45983
C	371	HIS	-	expression tag	UNP P45983
F	364	LEU	-	expression tag	UNP P45983
F	365	GLU	-	expression tag	UNP P45983
F	366	HIS	-	expression tag	UNP P45983
F	367	HIS	-	expression tag	UNP P45983
F	368	HIS	-	expression tag	UNP P45983
F	369	HIS	-	expression tag	UNP P45983
F	370	HIS	-	expression tag	UNP P45983
F	371	HIS	-	expression tag	UNP P45983

- Molecule 2 is a protein called Dual specificity protein phosphatase 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	141	Total	C	N	O	S	0	0	0
			1121	719	191	202	9			
2	B	141	Total	C	N	O	S	0	1	0
			1129	724	194	202	9			
2	D	142	Total	C	N	O	S	0	0	0
			1130	725	193	203	9			
2	H	143	Total	C	N	O	S	0	0	0
			1138	729	195	205	9			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	135	MET	-	expression tag	UNP Q9BY84
G	136	GLY	-	expression tag	UNP Q9BY84
G	137	SER	-	expression tag	UNP Q9BY84
G	138	SER	-	expression tag	UNP Q9BY84
G	139	HIS	-	expression tag	UNP Q9BY84
G	140	HIS	-	expression tag	UNP Q9BY84
G	141	HIS	-	expression tag	UNP Q9BY84
G	142	HIS	-	expression tag	UNP Q9BY84
G	143	HIS	-	expression tag	UNP Q9BY84
G	144	HIS	-	expression tag	UNP Q9BY84
G	145	SER	-	expression tag	UNP Q9BY84
G	146	SER	-	expression tag	UNP Q9BY84
G	147	GLY	-	expression tag	UNP Q9BY84
G	148	LEU	-	expression tag	UNP Q9BY84
G	149	VAL	-	expression tag	UNP Q9BY84

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Chain	Residue	Modelled	Actual	Comment	Reference
G	150	PRO	-	expression tag	UNP Q9BY84
G	151	ARG	-	expression tag	UNP Q9BY84
G	152	GLY	-	expression tag	UNP Q9BY84
G	153	SER	-	expression tag	UNP Q9BY84
G	154	HIS	-	expression tag	UNP Q9BY84
G	155	MET	-	expression tag	UNP Q9BY84
B	135	MET	-	expression tag	UNP Q9BY84
B	136	GLY	-	expression tag	UNP Q9BY84
B	137	SER	-	expression tag	UNP Q9BY84
B	138	SER	-	expression tag	UNP Q9BY84
B	139	HIS	-	expression tag	UNP Q9BY84
B	140	HIS	-	expression tag	UNP Q9BY84
B	141	HIS	-	expression tag	UNP Q9BY84
B	142	HIS	-	expression tag	UNP Q9BY84
B	143	HIS	-	expression tag	UNP Q9BY84
B	144	HIS	-	expression tag	UNP Q9BY84
B	145	SER	-	expression tag	UNP Q9BY84
B	146	SER	-	expression tag	UNP Q9BY84
B	147	GLY	-	expression tag	UNP Q9BY84
B	148	LEU	-	expression tag	UNP Q9BY84
B	149	VAL	-	expression tag	UNP Q9BY84
B	150	PRO	-	expression tag	UNP Q9BY84
B	151	ARG	-	expression tag	UNP Q9BY84
B	152	GLY	-	expression tag	UNP Q9BY84
B	153	SER	-	expression tag	UNP Q9BY84
B	154	HIS	-	expression tag	UNP Q9BY84
B	155	MET	-	expression tag	UNP Q9BY84
D	135	MET	-	expression tag	UNP Q9BY84
D	136	GLY	-	expression tag	UNP Q9BY84
D	137	SER	-	expression tag	UNP Q9BY84
D	138	SER	-	expression tag	UNP Q9BY84
D	139	HIS	-	expression tag	UNP Q9BY84
D	140	HIS	-	expression tag	UNP Q9BY84
D	141	HIS	-	expression tag	UNP Q9BY84
D	142	HIS	-	expression tag	UNP Q9BY84
D	143	HIS	-	expression tag	UNP Q9BY84
D	144	HIS	-	expression tag	UNP Q9BY84
D	145	SER	-	expression tag	UNP Q9BY84
D	146	SER	-	expression tag	UNP Q9BY84
D	147	GLY	-	expression tag	UNP Q9BY84
D	148	LEU	-	expression tag	UNP Q9BY84
D	149	VAL	-	expression tag	UNP Q9BY84

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Chain	Residue	Modelled	Actual	Comment	Reference
D	150	PRO	-	expression tag	UNP Q9BY84
D	151	ARG	-	expression tag	UNP Q9BY84
D	152	GLY	-	expression tag	UNP Q9BY84
D	153	SER	-	expression tag	UNP Q9BY84
D	154	HIS	-	expression tag	UNP Q9BY84
D	155	MET	-	expression tag	UNP Q9BY84
H	135	MET	-	expression tag	UNP Q9BY84
H	136	GLY	-	expression tag	UNP Q9BY84
H	137	SER	-	expression tag	UNP Q9BY84
H	138	SER	-	expression tag	UNP Q9BY84
H	139	HIS	-	expression tag	UNP Q9BY84
H	140	HIS	-	expression tag	UNP Q9BY84
H	141	HIS	-	expression tag	UNP Q9BY84
H	142	HIS	-	expression tag	UNP Q9BY84
H	143	HIS	-	expression tag	UNP Q9BY84
H	144	HIS	-	expression tag	UNP Q9BY84
H	145	SER	-	expression tag	UNP Q9BY84
H	146	SER	-	expression tag	UNP Q9BY84
H	147	GLY	-	expression tag	UNP Q9BY84
H	148	LEU	-	expression tag	UNP Q9BY84
H	149	VAL	-	expression tag	UNP Q9BY84
H	150	PRO	-	expression tag	UNP Q9BY84
H	151	ARG	-	expression tag	UNP Q9BY84
H	152	GLY	-	expression tag	UNP Q9BY84
H	153	SER	-	expression tag	UNP Q9BY84
H	154	HIS	-	expression tag	UNP Q9BY84
H	155	MET	-	expression tag	UNP Q9BY84

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0

- Molecule 4 is water.

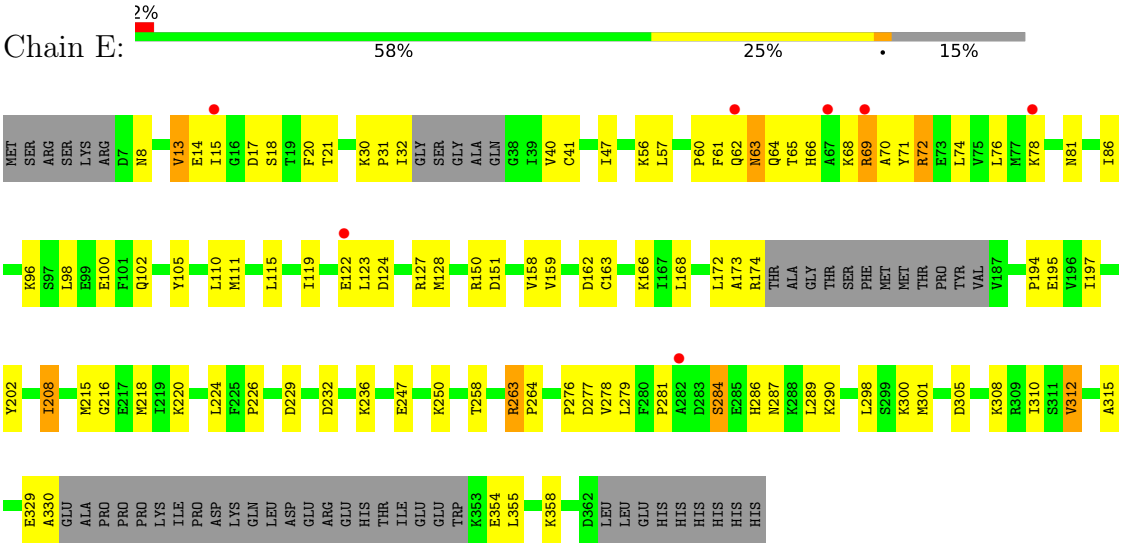
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	81	Total O 81 81	0	0
4	G	23	Total O 23 23	0	0
4	A	71	Total O 71 71	0	0
4	B	43	Total O 43 43	0	0
4	C	55	Total O 55 55	0	0
4	D	20	Total O 20 20	0	0
4	F	50	Total O 50 50	0	0
4	H	13	Total O 13 13	0	0

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.

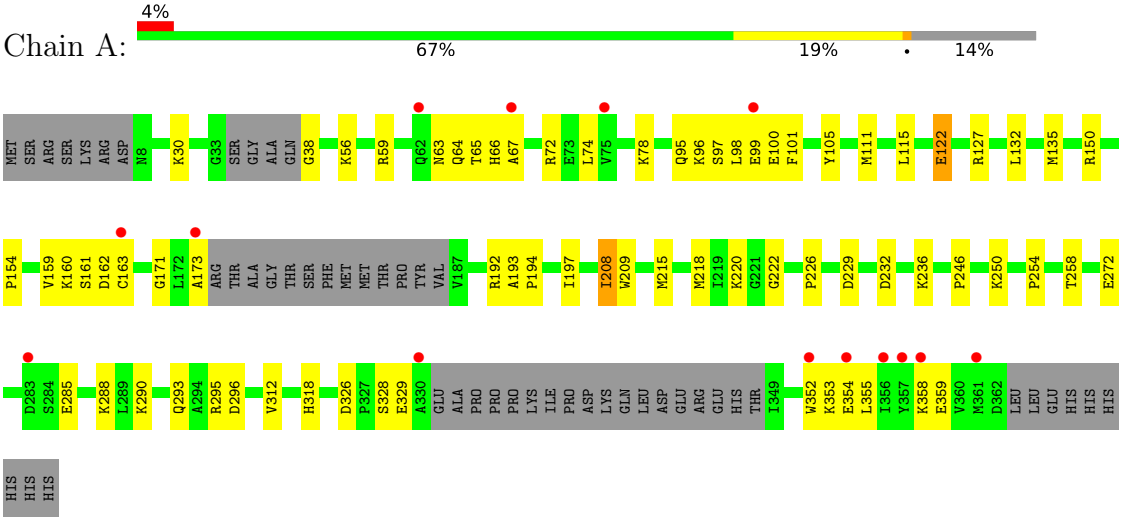
• Molecule 1: Mitogen-activated protein kinase 8

Chain E:



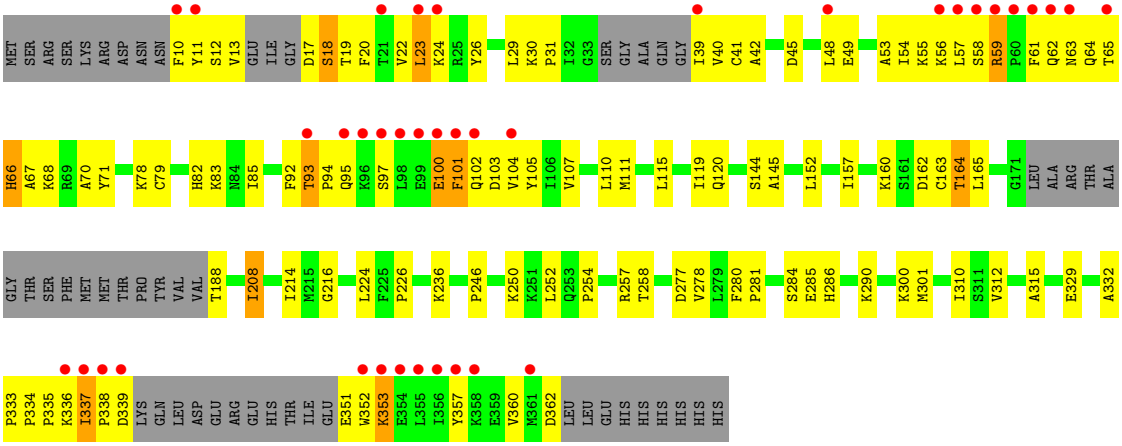
• Molecule 1: Mitogen-activated protein kinase 8

Chain A:



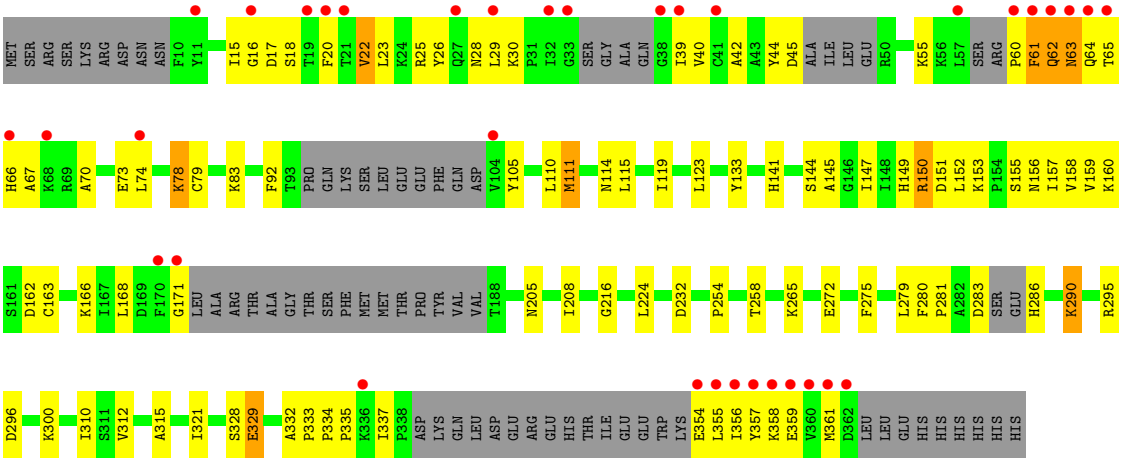
• Molecule 1: Mitogen-activated protein kinase 8

Chain C:



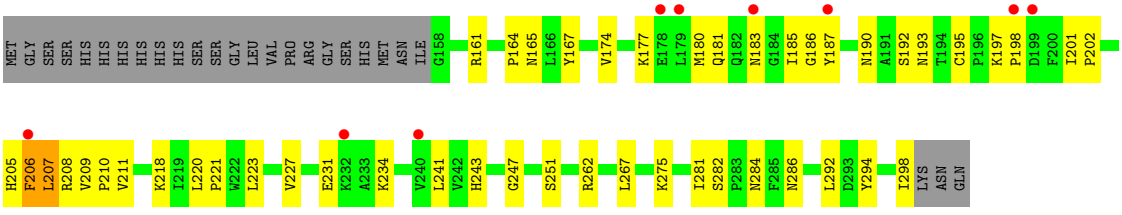
• Molecule 1: Mitogen-activated protein kinase 8

Chain F:



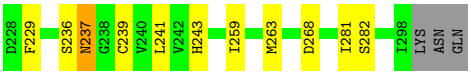
• Molecule 2: Dual specificity protein phosphatase 16

Chain G:

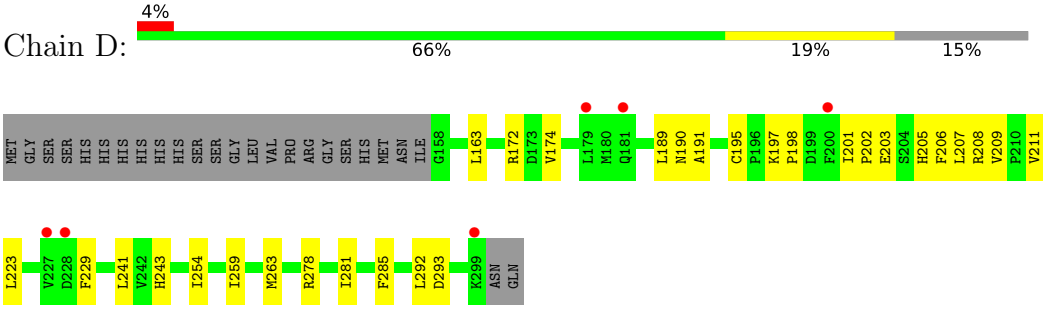


• Molecule 2: Dual specificity protein phosphatase 16

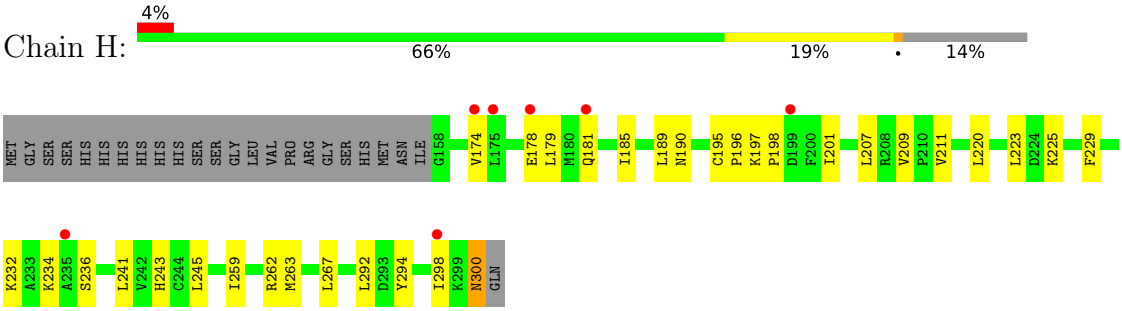
Chain B:



• Molecule 2: Dual specificity protein phosphatase 16



• Molecule 2: Dual specificity protein phosphatase 16



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.15Å 74.85Å 134.81Å 76.94° 84.32° 67.44°	Depositor
Resolution (Å)	38.02 – 2.40 38.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	83.8 (38.02-2.40) 83.5 (38.02-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.35 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.217 , 0.239 0.219 , 0.240	Depositor DCC
R_{free} test set	3406 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14988	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL

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	0.63	0/2636	0.75	0/3559
1	C	0.63	0/2622	0.75	0/3542
1	E	1.10	0/2603	0.79	0/3514
1	F	0.71	0/2465	0.73	0/3325
2	B	0.69	0/1156	0.74	0/1561
2	D	0.61	0/1154	0.71	0/1558
2	G	0.94	0/1145	0.82	0/1547
2	H	0.52	0/1162	0.70	0/1569
All	All	0.77	0/14943	0.75	0/20175

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

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	2582	0	2597	51	0
1	C	2565	0	2572	144	0
1	E	2551	0	2569	96	0
1	F	2412	0	2431	82	0
2	B	1129	0	1154	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1130	0	1154	36	0
2	G	1121	0	1141	71	0
2	H	1138	0	1160	21	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	71	0	0	6	0
4	B	43	0	0	1	0
4	C	55	0	0	3	0
4	D	20	0	0	2	0
4	E	81	0	0	5	0
4	F	50	0	0	2	0
4	G	23	0	0	2	0
4	H	13	0	0	0	0
All	All	14988	0	14778	520	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 18.

The worst 5 of 520 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)
2:G:207:LEU:HD12	2:G:208:ARG:N	1.31	1.40
1:C:63:ASN:CB	1:C:65:THR:HG22	1.71	1.19
1:C:101:PHE:CE2	1:C:357:TYR:HB2	1.82	1.14
2:B:198:PRO:HG2	2:B:201:ILE:HB	1.27	1.12
1:C:63:ASN:HB2	1:C:65:THR:HG22	1.27	1.10

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	312/371 (84%)	306 (98%)	6 (2%)	0	100	100
1	C	308/371 (83%)	299 (97%)	9 (3%)	0	100	100
1	E	309/371 (83%)	294 (95%)	15 (5%)	0	100	100
1	F	285/371 (77%)	276 (97%)	9 (3%)	0	100	100
2	B	140/167 (84%)	132 (94%)	8 (6%)	0	100	100
2	D	140/167 (84%)	135 (96%)	5 (4%)	0	100	100
2	G	139/167 (83%)	131 (94%)	8 (6%)	0	100	100
2	H	141/167 (84%)	137 (97%)	4 (3%)	0	100	100
All	All	1774/2152 (82%)	1710 (96%)	64 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	285/333 (86%)	276 (97%)	9 (3%)	39	59
1	C	283/333 (85%)	266 (94%)	17 (6%)	19	31
1	E	282/333 (85%)	261 (93%)	21 (7%)	13	22
1	F	266/333 (80%)	248 (93%)	18 (7%)	16	25
2	B	127/149 (85%)	121 (95%)	6 (5%)	26	42
2	D	127/149 (85%)	125 (98%)	2 (2%)	62	79
2	G	126/149 (85%)	123 (98%)	3 (2%)	49	68
2	H	128/149 (86%)	122 (95%)	6 (5%)	26	42
All	All	1624/1928 (84%)	1542 (95%)	82 (5%)	24	40

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	293	ASP
1	F	290	LYS

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Mol	Chain	Res	Type
1	F	22	VAL
1	F	111	MET
1	F	361	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	C	120	GLN
1	F	62	GLN
2	D	190	ASN
2	G	183	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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, 95^{th} 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	320/371 (86%)	0.03	14 (4%) 34 33	20, 33, 92, 159	0
1	C	318/371 (85%)	0.36	38 (11%) 4 4	22, 40, 106, 170	0
1	E	317/371 (85%)	0.01	7 (2%) 62 60	23, 34, 90, 159	0
1	F	300/371 (80%)	0.42	35 (11%) 4 4	10, 41, 100, 158	0
2	B	141/167 (84%)	-0.13	4 (2%) 53 51	14, 33, 73, 86	0
2	D	142/167 (85%)	0.11	6 (4%) 36 35	24, 50, 80, 90	0
2	G	141/167 (84%)	0.20	9 (6%) 19 18	20, 47, 88, 98	0
2	H	143/167 (85%)	0.16	7 (4%) 29 28	24, 49, 82, 93	0
All	All	1822/2152 (84%)	0.17	120 (6%) 18 17	10, 39, 92, 170	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	38	GLY	11.1
1	F	61	PHE	7.9
1	F	62	GLN	6.6
1	F	356	ILE	6.1
1	F	357	TYR	5.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
3	CL	B	401	1/1	0.93	0.21	30,30,30,30	0
3	CL	H	401	1/1	0.97	0.09	30,30,30,30	0
3	CL	D	401	1/1	0.98	0.11	30,30,30,30	0
3	CL	G	401	1/1	0.98	0.14	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.