



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:15 PM GMT

PDB ID : 1WMK  
Title : Human death-associated kinase DRP-1, mutant S308D d40  
Authors : Kursula, P.; Shani, G.; Kimchi, A.; Wilmanns, M.  
Deposited on : 2004-07-11  
Resolution : 3.60 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](mailto: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.

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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

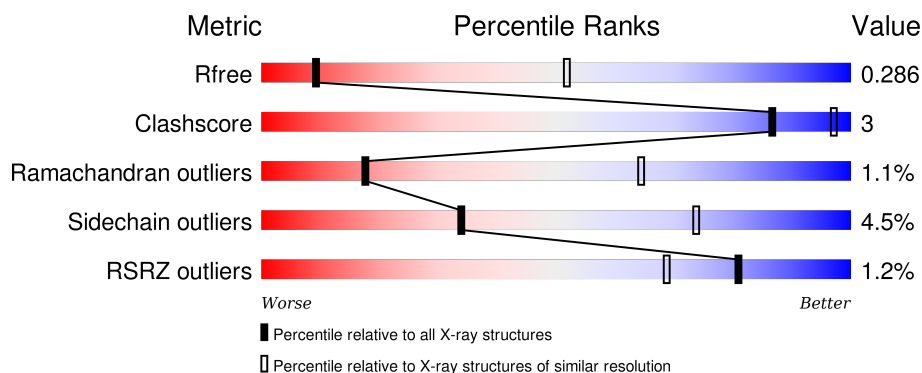
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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  $\geq 3$ , 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	321	
1	B	321	
1	C	321	
1	D	321	
1	E	321	

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Mol	Chain	Length	Quality of chain
1	F	321	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>81%</div><div>12%</div><div>• 6%</div></div></div>
1	G	321	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>85%</div><div>10%</div><div>• •</div></div></div>
1	H	321	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>82%</div><div>11%</div><div>• 5%</div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19951 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 Death-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2467	1578	421	464	4			
1	E	313	Total	C	N	O	S	0	0	0
			2517	1608	431	474	4			
1	C	303	Total	C	N	O	S	0	0	0
			2467	1578	421	464	4			
1	B	314	Total	C	N	O	S	0	0	0
			2522	1611	432	475	4			
1	F	303	Total	C	N	O	S	0	0	0
			2467	1578	421	464	4			
1	D	314	Total	C	N	O	S	0	0	0
			2522	1611	432	475	4			
1	H	304	Total	C	N	O	S	0	0	0
			2472	1581	422	465	4			
1	G	313	Total	C	N	O	S	0	0	0
			2517	1608	431	474	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	CLONING ARTIFACT	UNP Q9UIK4
A	308	ASP	SER	ENGINEERED	UNP Q9UIK4
B	0	GLY	-	CLONING ARTIFACT	UNP Q9UIK4
B	308	ASP	SER	ENGINEERED	UNP Q9UIK4
C	0	GLY	-	CLONING ARTIFACT	UNP Q9UIK4
C	308	ASP	SER	ENGINEERED	UNP Q9UIK4
D	0	GLY	-	CLONING ARTIFACT	UNP Q9UIK4
D	308	ASP	SER	ENGINEERED	UNP Q9UIK4
E	0	GLY	-	CLONING ARTIFACT	UNP Q9UIK4
E	308	ASP	SER	ENGINEERED	UNP Q9UIK4
F	0	GLY	-	CLONING ARTIFACT	UNP Q9UIK4
F	308	ASP	SER	ENGINEERED	UNP Q9UIK4
G	0	GLY	-	CLONING ARTIFACT	UNP Q9UIK4

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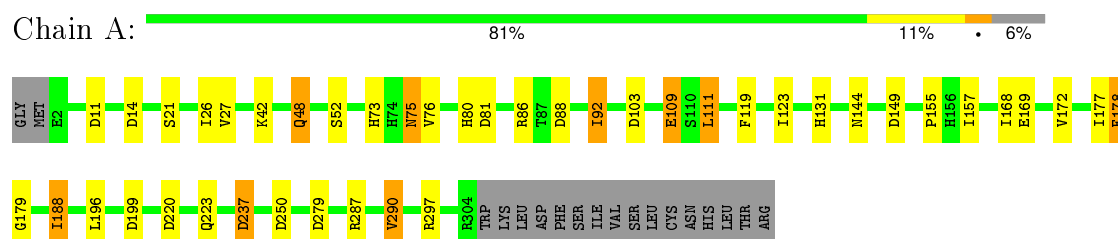
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Chain	Residue	Modelled	Actual	Comment	Reference
G	308	ASP	SER	ENGINEERED	UNP Q9UIK4
H	0	GLY	-	CLONING ARTIFACT	UNP Q9UIK4
H	308	ASP	SER	ENGINEERED	UNP Q9UIK4

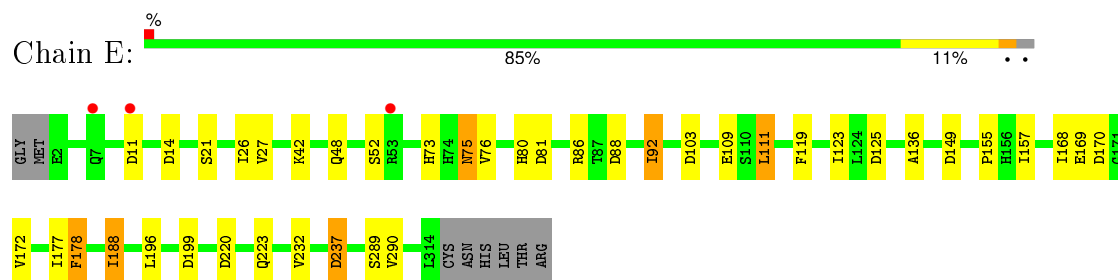
### 3 Residue-property plots [i](#)

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.

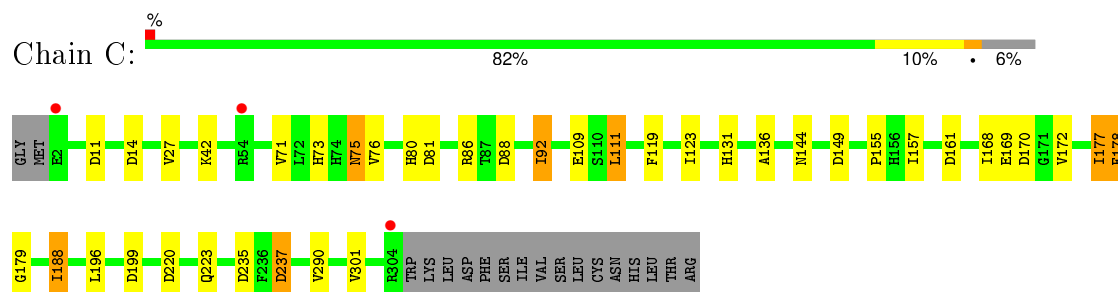
#### • Molecule 1: Death-associated protein kinase 2



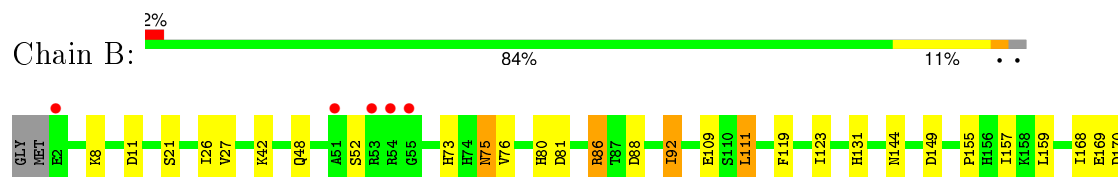
#### • Molecule 1: Death-associated protein kinase 2

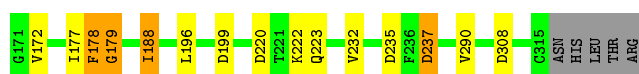


#### • Molecule 1: Death-associated protein kinase 2

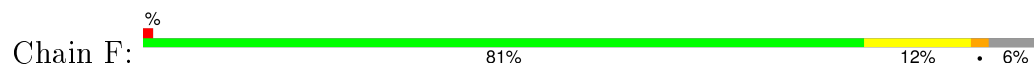


#### • Molecule 1: Death-associated protein kinase 2

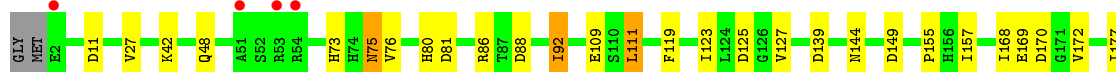
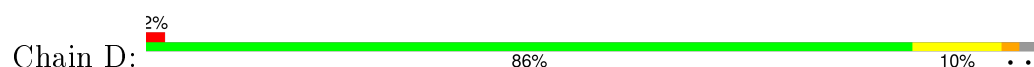




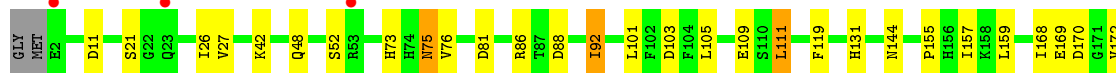
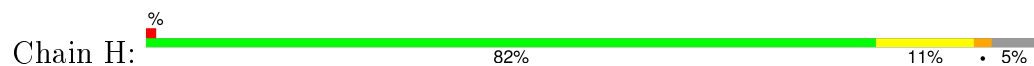
- Molecule 1: Death-associated protein kinase 2



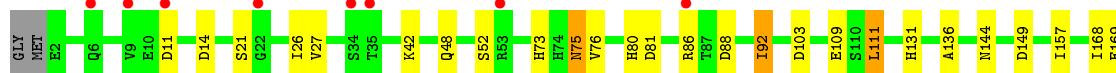
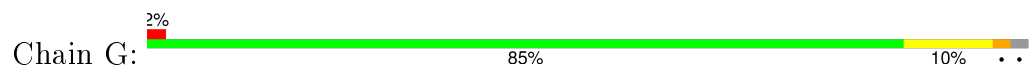
- Molecule 1: Death-associated protein kinase 2



- Molecule 1: Death-associated protein kinase 2



- Molecule 1: Death-associated protein kinase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.19Å 143.29Å 255.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60 19.99 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.60) 100.0 (19.99-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 3.62Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, $R_{free}$	0.276 , 0.296 0.266 , 0.286	Depositor DCC
$R_{free}$ test set	1864 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.2	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 64.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 37261 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	19951	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

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	0.34	0/2514	0.65	11/3391 (0.3%)
1	B	0.34	0/2569	0.66	9/3468 (0.3%)
1	C	0.34	0/2514	0.65	10/3391 (0.3%)
1	D	0.34	0/2569	0.65	11/3468 (0.3%)
1	E	0.33	0/2564	0.65	11/3461 (0.3%)
1	F	0.31	0/2514	0.64	10/3391 (0.3%)
1	G	0.32	0/2564	0.64	11/3461 (0.3%)
1	H	0.34	0/2519	0.65	10/3398 (0.3%)
All	All	0.33	0/20327	0.65	83/27429 (0.3%)

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	CB-CG-OD2	6.82	124.44	118.30
1	F	81	ASP	CB-CG-OD2	6.67	124.31	118.30
1	C	81	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	199	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	81	ASP	CB-CG-OD2	6.38	124.05	118.30
1	E	81	ASP	CB-CG-OD2	6.38	124.04	118.30
1	H	81	ASP	CB-CG-OD2	6.37	124.03	118.30
1	G	81	ASP	CB-CG-OD2	6.29	123.96	118.30
1	D	237	ASP	CB-CG-OD2	6.05	123.75	118.30
1	F	103	ASP	CB-CG-OD2	6.03	123.73	118.30
1	D	81	ASP	CB-CG-OD2	6.01	123.71	118.30
1	E	103	ASP	CB-CG-OD2	5.89	123.60	118.30
1	H	199	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	220	ASP	CB-CG-OD2	5.76	123.48	118.30
1	E	237	ASP	CB-CG-OD2	5.61	123.35	118.30
1	G	103	ASP	CB-CG-OD2	5.60	123.34	118.30
1	H	88	ASP	CB-CG-OD2	5.58	123.33	118.30
1	C	220	ASP	CB-CG-OD2	5.56	123.31	118.30
1	G	237	ASP	CB-CG-OD2	5.56	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	237	ASP	CB-CG-OD2	5.55	123.29	118.30
1	D	250	ASP	CB-CG-OD2	5.53	123.28	118.30
1	F	199	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	88	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	88	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	220	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	14	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	11	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	237	ASP	CB-CG-OD2	5.42	123.18	118.30
1	G	220	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	149	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	250	ASP	CB-CG-OD2	5.40	123.16	118.30
1	H	279	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	199	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	149	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	220	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	170	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	149	ASP	CB-CG-OD2	5.36	123.13	118.30
1	G	149	ASP	CB-CG-OD2	5.36	123.12	118.30
1	E	88	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	199	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	103	ASP	CB-CG-OD2	5.35	123.11	118.30
1	H	250	ASP	CB-CG-OD2	5.34	123.11	118.30
1	G	88	ASP	CB-CG-OD2	5.34	123.10	118.30
1	E	11	ASP	CB-CG-OD2	5.34	123.10	118.30
1	E	170	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	199	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	11	ASP	CB-CG-OD2	5.31	123.08	118.30
1	H	237	ASP	CB-CG-OD2	5.30	123.07	118.30
1	G	170	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	88	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	220	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	170	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	149	ASP	CB-CG-OD2	5.28	123.06	118.30
1	G	250	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	149	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	199	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	11	ASP	CB-CG-OD2	5.26	123.04	118.30
1	E	125	ASP	CB-CG-OD2	5.26	123.03	118.30
1	F	11	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	250	ASP	CB-CG-OD2	5.24	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	199	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	88	ASP	CB-CG-OD2	5.23	123.00	118.30
1	H	103	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	237	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	235	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	125	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	161	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	220	ASP	CB-CG-OD2	5.16	122.95	118.30
1	D	170	ASP	CB-CG-OD2	5.16	122.94	118.30
1	F	14	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	11	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	170	ASP	CB-CG-OD2	5.10	122.89	118.30
1	G	11	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	14	ASP	CB-CG-OD2	5.09	122.88	118.30
1	G	14	ASP	CB-CG-OD2	5.08	122.88	118.30
1	H	220	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	139	ASP	CB-CG-OD2	5.05	122.84	118.30
1	H	11	ASP	CB-CG-OD2	5.04	122.83	118.30
1	H	170	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	14	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	88	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	279	ASP	CB-CG-OD2	5.00	122.80	118.30

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	2467	0	2476	18	0
1	B	2522	0	2498	18	0
1	C	2467	0	2476	16	0
1	D	2522	0	2498	11	0
1	E	2517	0	2496	12	0
1	F	2467	0	2476	14	0
1	G	2517	0	2496	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2472	0	2478	13	0
All	All	19951	0	19894	107	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 (107) 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:C:235:ASP:OD2	1:D:254:LYS:NZ	2.30	0.64
1:D:75:ASN:ND2	1:D:157:ILE:O	2.31	0.64
1:A:287:ARG:HD3	1:B:8:LYS:HE2	1.81	0.63
1:E:178:PHE:HB2	1:E:188:ILE:HD12	1.83	0.60
1:F:178:PHE:HB2	1:F:188:ILE:HD12	1.84	0.60
1:H:75:ASN:ND2	1:H:157:ILE:O	2.34	0.60
1:A:178:PHE:HB2	1:A:188:ILE:HD12	1.85	0.59
1:A:109:GLU:HG3	1:B:48:GLN:CD	2.22	0.59
1:E:119:PHE:O	1:E:123:ILE:HD12	2.03	0.58
1:C:178:PHE:HB2	1:C:188:ILE:HD12	1.85	0.58
1:G:178:PHE:HB2	1:G:188:ILE:HD12	1.85	0.58
1:B:178:PHE:HB2	1:B:188:ILE:HD12	1.86	0.58
1:C:169:GLU:HB2	1:C:172:VAL:HB	1.87	0.57
1:A:297:ARG:NH1	1:C:301:VAL:HG13	2.20	0.57
1:E:169:GLU:HB2	1:E:172:VAL:HB	1.87	0.56
1:H:178:PHE:HB2	1:H:188:ILE:HD12	1.89	0.55
1:A:27:VAL:HG22	1:A:42:LYS:HG3	1.88	0.55
1:D:169:GLU:HB2	1:D:172:VAL:HB	1.87	0.55
1:D:27:VAL:HG22	1:D:42:LYS:HG3	1.89	0.55
1:H:73:HIS:HB3	1:H:76:VAL:HG22	1.89	0.54
1:D:178:PHE:HB2	1:D:188:ILE:HD12	1.88	0.54
1:G:169:GLU:HB2	1:G:172:VAL:HB	1.89	0.54
1:A:290:VAL:HG13	1:B:86:ARG:HH12	1.72	0.54
1:B:169:GLU:HB2	1:B:172:VAL:HB	1.89	0.54
1:C:119:PHE:O	1:C:123:ILE:HD12	2.08	0.54
1:A:109:GLU:HG3	1:B:48:GLN:NE2	2.23	0.53
1:A:169:GLU:HB2	1:A:172:VAL:HB	1.90	0.53
1:H:27:VAL:HG22	1:H:42:LYS:HG3	1.91	0.53
1:A:119:PHE:O	1:A:123:ILE:HD12	2.09	0.52
1:C:27:VAL:HG22	1:C:42:LYS:HG3	1.90	0.52
1:F:27:VAL:HG22	1:F:42:LYS:HG3	1.92	0.52
1:C:73:HIS:HB3	1:C:76:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:GLU:HB2	1:F:172:VAL:HB	1.91	0.51
1:A:80:HIS:HB3	1:A:92:ILE:HG22	1.92	0.51
1:B:27:VAL:HG22	1:B:42:LYS:HG3	1.92	0.51
1:H:169:GLU:HB2	1:H:172:VAL:HB	1.92	0.51
1:G:27:VAL:HG22	1:G:42:LYS:HG3	1.92	0.50
1:E:73:HIS:HB3	1:E:76:VAL:HG22	1.93	0.50
1:D:73:HIS:HB3	1:D:76:VAL:HG22	1.94	0.50
1:A:73:HIS:HB3	1:A:76:VAL:HG22	1.94	0.49
1:A:21:SER:HB2	1:A:26:ILE:HG13	1.93	0.49
1:E:75:ASN:ND2	1:E:157:ILE:O	2.44	0.49
1:B:73:HIS:HB3	1:B:76:VAL:HG22	1.93	0.49
1:G:73:HIS:HB3	1:G:76:VAL:HG22	1.94	0.49
1:F:73:HIS:HB3	1:F:76:VAL:HG22	1.94	0.48
1:A:119:PHE:HE2	1:A:155:PRO:HD2	1.78	0.48
1:F:119:PHE:O	1:F:123:ILE:HD12	2.14	0.48
1:E:27:VAL:HG22	1:E:42:LYS:HG3	1.95	0.48
1:H:119:PHE:HE2	1:H:155:PRO:HD2	1.78	0.47
1:C:80:HIS:HB3	1:C:92:ILE:HG22	1.97	0.47
1:G:80:HIS:HB3	1:G:92:ILE:HG22	1.97	0.47
1:F:75:ASN:ND2	1:F:157:ILE:O	2.47	0.47
1:D:119:PHE:HE2	1:D:155:PRO:HD2	1.80	0.46
1:D:119:PHE:O	1:D:123:ILE:HD12	2.15	0.46
1:G:131:HIS:CD2	1:G:196:LEU:HB3	2.51	0.46
1:G:75:ASN:ND2	1:G:157:ILE:O	2.48	0.46
1:D:80:HIS:HB3	1:D:92:ILE:HG22	1.98	0.46
1:B:119:PHE:O	1:B:123:ILE:HD12	2.17	0.45
1:F:101:LEU:O	1:F:105:LEU:HG	2.16	0.45
1:C:119:PHE:HE2	1:C:155:PRO:HD2	1.81	0.45
1:C:178:PHE:HB3	1:C:179:GLY:H	1.62	0.45
1:H:178:PHE:HB3	1:H:179:GLY:H	1.63	0.45
1:A:131:HIS:CD2	1:A:196:LEU:HB3	2.52	0.45
1:B:119:PHE:HE2	1:B:155:PRO:HD2	1.82	0.45
1:D:178:PHE:HB3	1:D:179:GLY:H	1.60	0.44
1:H:101:LEU:O	1:H:105:LEU:HG	2.16	0.44
1:E:136:ALA:HB2	1:E:196:LEU:HD23	1.99	0.44
1:B:131:HIS:CD2	1:B:196:LEU:HB3	2.53	0.44
1:B:48:GLN:HB2	1:B:52:SER:OG	2.17	0.44
1:E:80:HIS:HB3	1:E:92:ILE:HG22	1.99	0.44
1:A:48:GLN:HB2	1:A:52:SER:OG	2.18	0.44
1:G:178:PHE:HB3	1:G:179:GLY:H	1.64	0.44
1:H:21:SER:HB2	1:H:26:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HB3	1:B:179:GLY:H	1.64	0.44
1:F:48:GLN:HB2	1:F:52:SER:OG	2.18	0.44
1:B:75:ASN:ND2	1:B:157:ILE:O	2.51	0.43
1:E:92:ILE:N	1:E:92:ILE:CD1	2.81	0.43
1:E:21:SER:HB2	1:E:26:ILE:HG13	2.00	0.43
1:H:131:HIS:CD2	1:H:196:LEU:HB3	2.53	0.43
1:F:80:HIS:HB3	1:F:92:ILE:HG22	2.01	0.43
1:E:48:GLN:HB2	1:E:52:SER:OG	2.19	0.43
1:A:92:ILE:N	1:A:92:ILE:CD1	2.81	0.43
1:A:178:PHE:HB3	1:A:179:GLY:H	1.60	0.43
1:H:76:VAL:HG12	1:H:159:LEU:HD12	2.01	0.43
1:C:92:ILE:CD1	1:C:92:ILE:N	2.81	0.43
1:G:92:ILE:CD1	1:G:92:ILE:N	2.81	0.42
1:F:21:SER:HB2	1:F:26:ILE:HG13	2.01	0.42
1:A:75:ASN:ND2	1:A:157:ILE:O	2.53	0.42
1:H:48:GLN:HB2	1:H:52:SER:OG	2.19	0.42
1:F:131:HIS:CD2	1:F:196:LEU:HB3	2.54	0.42
1:G:136:ALA:HB2	1:G:196:LEU:HD23	2.00	0.42
1:E:119:PHE:HE2	1:E:155:PRO:HD2	1.85	0.42
1:H:92:ILE:N	1:H:92:ILE:CD1	2.83	0.42
1:C:75:ASN:ND2	1:C:157:ILE:O	2.51	0.41
1:B:80:HIS:HB3	1:B:92:ILE:HG22	2.02	0.41
1:C:177:ILE:HG22	1:B:222:LYS:HE2	2.01	0.41
1:C:131:HIS:CD2	1:C:196:LEU:HB3	2.56	0.41
1:F:154:ILE:HA	1:F:155:PRO:HD3	1.90	0.41
1:G:48:GLN:HB2	1:G:52:SER:OG	2.21	0.41
1:G:21:SER:HB2	1:G:26:ILE:HG13	2.02	0.41
1:B:21:SER:HB2	1:B:26:ILE:HG13	2.02	0.41
1:B:76:VAL:HG12	1:B:159:LEU:HD12	2.03	0.40
1:F:119:PHE:HE2	1:F:155:PRO:HD2	1.85	0.40
1:D:123:ILE:O	1:D:127:VAL:HG23	2.21	0.40
1:C:136:ALA:HB2	1:C:196:LEU:HD23	2.02	0.40
1:F:202:SER:O	1:F:206:ILE:HG12	2.20	0.40
1:C:71:VAL:CG1	1:C:76:VAL:HG21	2.52	0.40

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	301/321 (94%)	273 (91%)	25 (8%)	3 (1%)	19	66
1	B	312/321 (97%)	282 (90%)	25 (8%)	5 (2%)	12	56
1	C	301/321 (94%)	274 (91%)	25 (8%)	2 (1%)	26	72
1	D	312/321 (97%)	282 (90%)	26 (8%)	4 (1%)	15	60
1	E	311/321 (97%)	281 (90%)	27 (9%)	3 (1%)	19	66
1	F	301/321 (94%)	274 (91%)	25 (8%)	2 (1%)	26	72
1	G	311/321 (97%)	281 (90%)	27 (9%)	3 (1%)	19	66
1	H	302/321 (94%)	269 (89%)	29 (10%)	4 (1%)	15	60
All	All	2451/2568 (95%)	2216 (90%)	209 (8%)	26 (1%)	17	64

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	111	LEU
1	E	86	ARG
1	E	111	LEU
1	C	86	ARG
1	C	111	LEU
1	B	86	ARG
1	B	111	LEU
1	F	86	ARG
1	F	111	LEU
1	D	86	ARG
1	D	111	LEU
1	H	86	ARG
1	H	111	LEU
1	G	86	ARG
1	G	111	LEU
1	D	306	LYS

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Mol	Chain	Res	Type
1	B	308	ASP
1	A	48	GLN
1	D	48	GLN
1	B	179	GLY
1	H	179	GLY
1	G	179	GLY
1	B	232	VAL
1	E	232	VAL
1	H	232	VAL

### 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	271/289 (94%)	259 (96%)	12 (4%)	35	74
1	B	271/289 (94%)	259 (96%)	12 (4%)	35	74
1	C	271/289 (94%)	259 (96%)	12 (4%)	35	74
1	D	271/289 (94%)	259 (96%)	12 (4%)	35	74
1	E	271/289 (94%)	259 (96%)	12 (4%)	35	74
1	F	271/289 (94%)	259 (96%)	12 (4%)	35	74
1	G	271/289 (94%)	258 (95%)	13 (5%)	31	72
1	H	271/289 (94%)	259 (96%)	12 (4%)	35	74
All	All	2168/2312 (94%)	2071 (96%)	97 (4%)	34	74

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	ILE
1	A	109	GLU
1	A	111	LEU
1	A	144	ASN
1	A	168	ILE

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Mol	Chain	Res	Type
1	A	177	ILE
1	A	178	PHE
1	A	188	ILE
1	A	223	GLN
1	A	237	ASP
1	A	290	VAL
1	E	75	ASN
1	E	92	ILE
1	E	109	GLU
1	E	111	LEU
1	E	168	ILE
1	E	177	ILE
1	E	178	PHE
1	E	188	ILE
1	E	223	GLN
1	E	237	ASP
1	E	289	SER
1	E	290	VAL
1	C	75	ASN
1	C	92	ILE
1	C	109	GLU
1	C	111	LEU
1	C	144	ASN
1	C	168	ILE
1	C	177	ILE
1	C	178	PHE
1	C	188	ILE
1	C	223	GLN
1	C	237	ASP
1	C	290	VAL
1	B	75	ASN
1	B	92	ILE
1	B	109	GLU
1	B	111	LEU
1	B	144	ASN
1	B	168	ILE
1	B	177	ILE
1	B	178	PHE
1	B	188	ILE
1	B	223	GLN
1	B	237	ASP
1	B	290	VAL

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Mol	Chain	Res	Type
1	F	75	ASN
1	F	92	ILE
1	F	109	GLU
1	F	111	LEU
1	F	144	ASN
1	F	168	ILE
1	F	177	ILE
1	F	178	PHE
1	F	188	ILE
1	F	223	GLN
1	F	237	ASP
1	F	290	VAL
1	D	75	ASN
1	D	92	ILE
1	D	109	GLU
1	D	111	LEU
1	D	144	ASN
1	D	168	ILE
1	D	177	ILE
1	D	178	PHE
1	D	188	ILE
1	D	223	GLN
1	D	237	ASP
1	D	290	VAL
1	H	75	ASN
1	H	92	ILE
1	H	109	GLU
1	H	111	LEU
1	H	144	ASN
1	H	168	ILE
1	H	177	ILE
1	H	178	PHE
1	H	188	ILE
1	H	223	GLN
1	H	237	ASP
1	H	290	VAL
1	G	75	ASN
1	G	92	ILE
1	G	109	GLU
1	G	111	LEU
1	G	144	ASN
1	G	168	ILE

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Mol	Chain	Res	Type
1	G	177	ILE
1	G	178	PHE
1	G	188	ILE
1	G	223	GLN
1	G	237	ASP
1	G	289	SER
1	G	290	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	144	ASN
1	A	223	GLN
1	A	267	GLN
1	E	74	HIS
1	E	144	ASN
1	E	223	GLN
1	C	74	HIS
1	C	144	ASN
1	B	74	HIS
1	B	80	HIS
1	B	144	ASN
1	B	223	GLN
1	F	74	HIS
1	F	144	ASN
1	F	267	GLN
1	D	74	HIS
1	D	144	ASN
1	D	223	GLN
1	D	267	GLN
1	H	74	HIS
1	H	144	ASN
1	H	223	GLN
1	H	267	GLN
1	G	74	HIS
1	G	144	ASN
1	G	223	GLN

### 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 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	303/321 (94%)	-0.57	0 <b>100</b> <b>100</b>	35, 115, 216, 226	0
1	B	314/321 (97%)	-0.49	5 (1%) 74 61	32, 116, 224, 226	0
1	C	303/321 (94%)	-0.50	3 (0%) 84 73	34, 122, 214, 226	0
1	D	314/321 (97%)	-0.47	6 (1%) 70 56	46, 131, 216, 226	0
1	E	313/321 (97%)	-0.39	3 (0%) 84 73	40, 129, 226, 226	0
1	F	303/321 (94%)	-0.33	2 (0%) 89 81	58, 159, 226, 226	0
1	G	313/321 (97%)	-0.39	8 (2%) 59 44	35, 135, 226, 226	0
1	H	304/321 (94%)	-0.53	3 (0%) 84 73	44, 124, 218, 226	0
All	All	2467/2568 (96%)	-0.46	30 (1%) 81 69	32, 129, 225, 226	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	53	ARG	5.7
1	B	54	ARG	5.2
1	G	11	ASP	4.8
1	B	2	GLU	4.4
1	H	2	GLU	4.2
1	B	53	ARG	3.8
1	H	23	GLN	3.6
1	E	7	GLN	3.3
1	D	54	ARG	3.2
1	D	2	GLU	3.1
1	G	35	THR	3.0
1	C	304	ARG	3.0
1	B	55	GLY	2.8
1	G	34	SER	2.7
1	C	2	GLU	2.7
1	B	51	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	308	ASP	2.7
1	G	53	ARG	2.5
1	H	53	ARG	2.5
1	F	243	GLN	2.5
1	G	22	GLY	2.4
1	C	54	ARG	2.4
1	E	53	ARG	2.4
1	F	49	SER	2.2
1	G	86	ARG	2.2
1	E	11	ASP	2.2
1	D	280	ASN	2.2
1	D	51	ALA	2.1
1	G	6	GLN	2.1
1	G	9	VAL	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.