



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:24 AM GMT

PDB ID : 3I6W
Title : Structure and Activation Mechanism of the CHK2 DNA-Damage Checkpoint Kinase
Authors : Pavletich, N.P.
Deposited on : 2009-07-07
Resolution : 3.25 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
<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

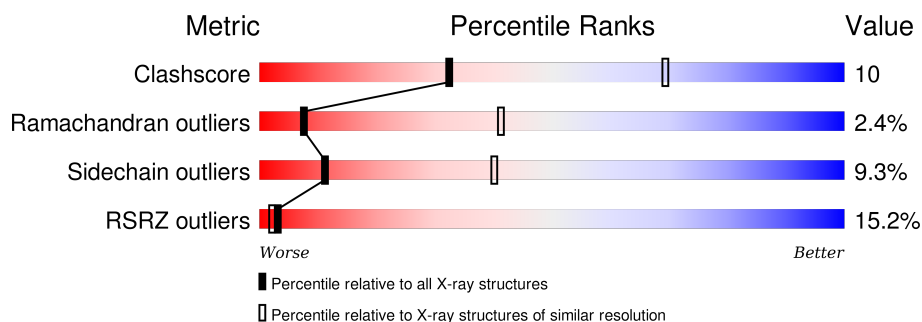
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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))
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	443	<div> <div>8%</div> <div>60% 19% 17%</div> </div>
1	B	443	<div> <div>9%</div> <div>63% 21% 14%</div> </div>
1	C	443	<div> <div>7%</div> <div>58% 21% 17%</div> </div>
1	D	443	<div> <div>13%</div> <div>63% 21% 14%</div> </div>
1	E	443	<div> <div>18%</div> <div>60% 20% 17%</div> </div>
1	F	443	<div> <div>21%</div> <div>65% 18% 14%</div> </div>
1	G	443	<div> <div>12%</div> <div>59% 20% 17%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	443	<div><div><div>15%</div><div>62%</div><div>22%</div><div>14%</div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24560 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 Chk2.

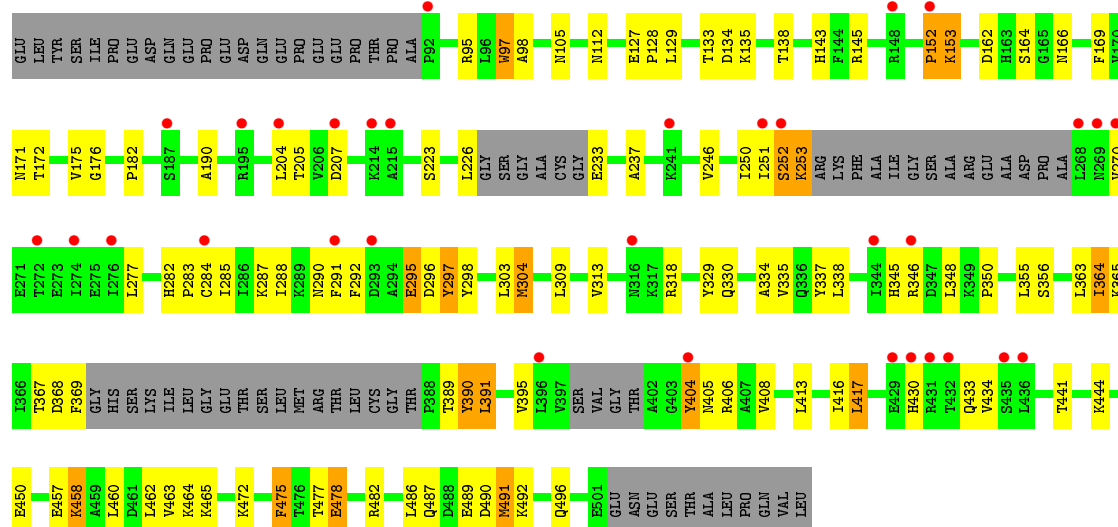
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			3022	1952	504	553	13			
1	B	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	C	368	Total	C	N	O	S	0	0	0
			3018	1950	503	552	13			
1	D	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	E	368	Total	C	N	O	S	0	0	0
			3018	1950	503	552	13			
1	F	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	G	369	Total	C	N	O	S	0	0	0
			3022	1952	504	553	13			
1	H	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			

There are 8 discrepancies between the modelled and reference sequences:

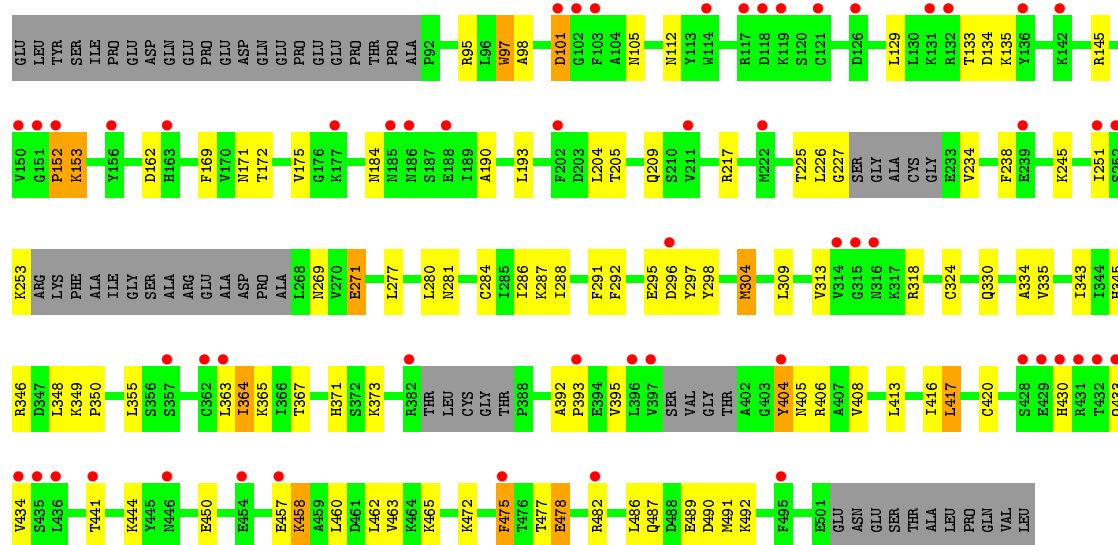
Chain	Residue	Modelled	Actual	Comment	Reference
A	249	ARG	LYS	engineered	UNP O96017
B	249	ARG	LYS	engineered	UNP O96017
C	249	ARG	LYS	engineered	UNP O96017
D	249	ARG	LYS	engineered	UNP O96017
E	249	ARG	LYS	engineered	UNP O96017
F	249	ARG	LYS	engineered	UNP O96017
G	249	ARG	LYS	engineered	UNP O96017
H	249	ARG	LYS	engineered	UNP O96017



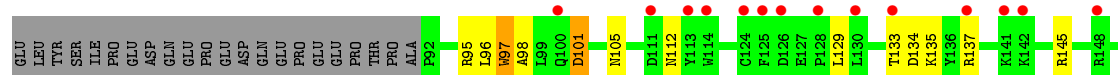
• Molecule 1: Serine/threonine-protein kinase Chk2

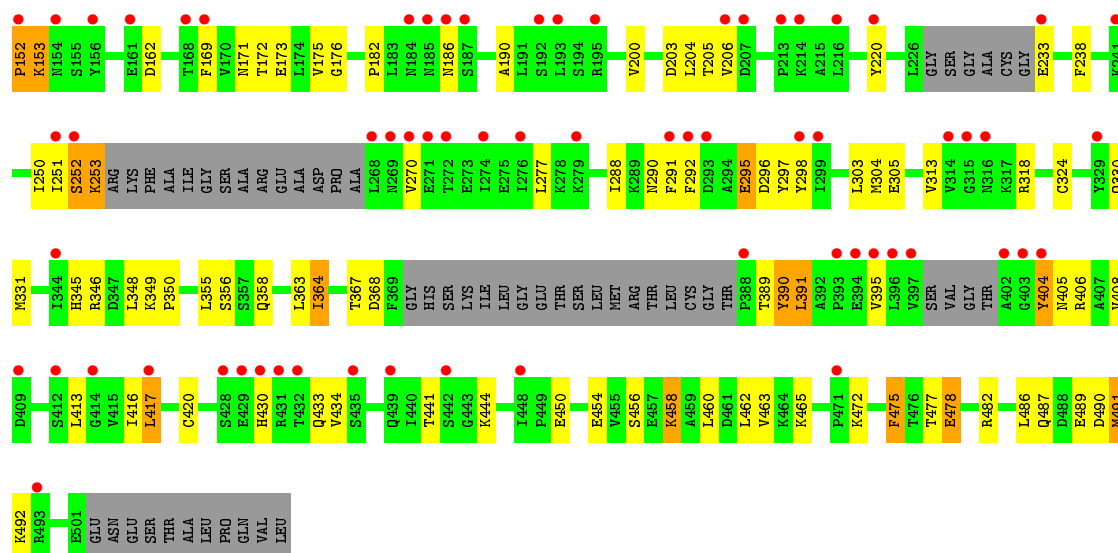


• Molecule 1: Serine/threonine-protein kinase Chk2

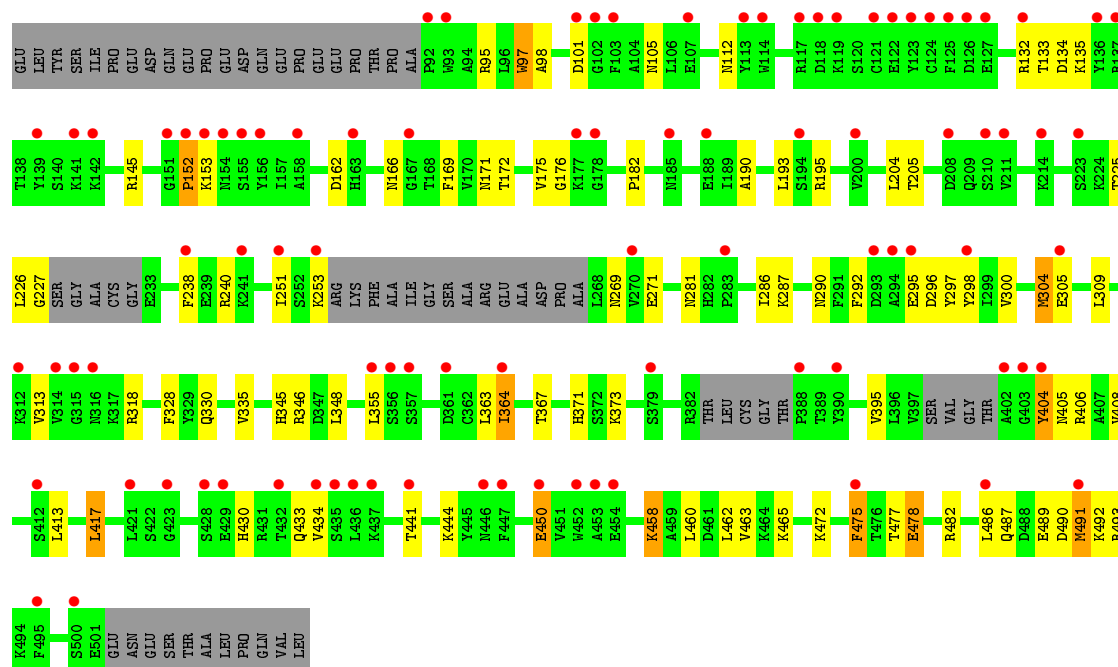


• Molecule 1: Serine/threonine-protein kinase Chk2

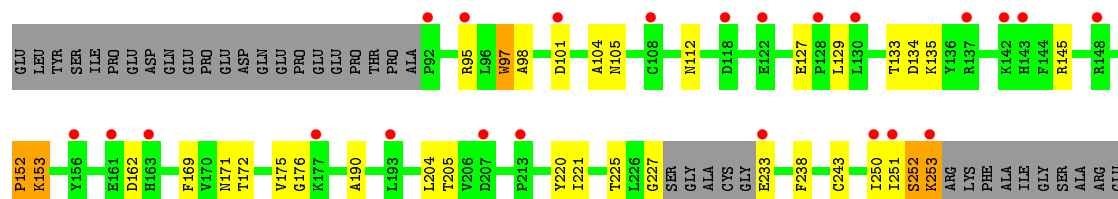


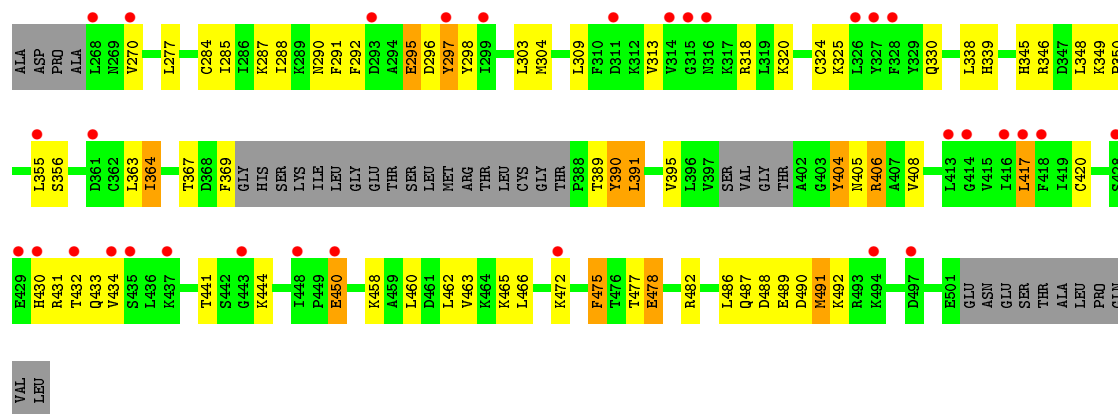


• Molecule 1: Serine/threonine-protein kinase Chk2

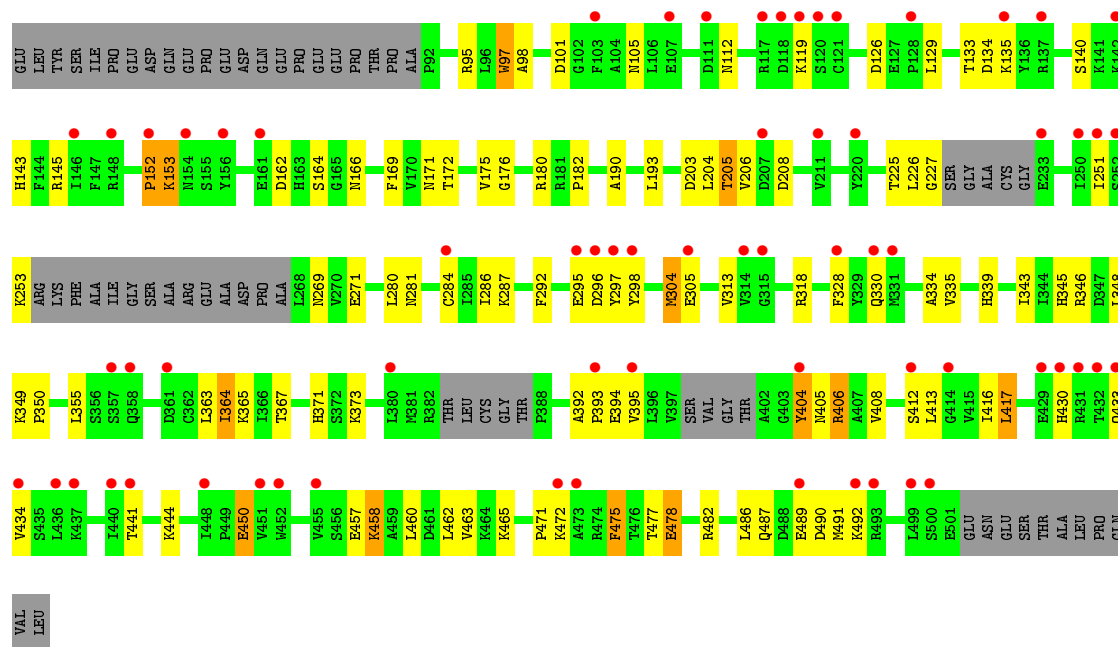


• Molecule 1: Serine/threonine-protein kinase Chk2





• Molecule 1: Serine/threonine-protein kinase Chk2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.20Å 114.70Å 123.00Å 84.10° 81.20° 80.70°	Depositor
Resolution (Å)	30.00 – 3.25 29.86 – 3.25	Depositor EDS
% Data completeness (in resolution range)	90.8 (30.00-3.25) 88.8 (29.86-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.251 , 0.287 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	120.4	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 172.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 60982 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24560	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/3087	0.59	0/4163
1	B	0.49	0/3186	0.60	1/4294 (0.0%)
1	C	0.55	0/3083	0.63	1/4158 (0.0%)
1	D	0.46	0/3186	0.60	1/4294 (0.0%)
1	E	0.44	0/3083	0.58	0/4158
1	F	0.41	0/3186	0.57	1/4294 (0.0%)
1	G	0.43	0/3087	0.58	1/4163 (0.0%)
1	H	0.40	0/3186	0.57	0/4294
All	All	0.46	0/25084	0.59	5/33818 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	LEU	CA-CB-CG	5.17	127.20	115.30
1	G	309	LEU	CA-CB-CG	5.12	127.07	115.30
1	C	309	LEU	CA-CB-CG	5.09	127.01	115.30
1	F	309	LEU	CA-CB-CG	5.05	126.92	115.30
1	D	309	LEU	CA-CB-CG	5.04	126.89	115.30

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	3022	0	3026	80	6
1	B	3120	0	3130	79	0
1	C	3018	0	3023	74	5
1	D	3120	0	3130	71	0
1	E	3018	0	3023	81	6
1	F	3120	0	3130	69	8
1	G	3022	0	3026	69	5
1	H	3120	0	3130	84	4
All	All	24560	0	24618	516	20

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 10.

The worst 5 of 516 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:A:129:LEU:HD23	1:D:193:LEU:CD2	1.47	1.44
1:A:129:LEU:CD2	1:D:193:LEU:HD21	1.52	1.40
1:F:132:ARG:CD	1:H:129:LEU:HD13	1.74	1.16
1:B:166:ASN:HD22	1:C:129:LEU:HB2	1.15	1.09
1:F:132:ARG:HD2	1:H:129:LEU:CD1	1.84	1.07

The worst 5 of 20 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:320:LYS:CD	1:H:457:GLU:OE2[1_455]	0.80	1.40
1:C:138:THR:CG2	1:C:496:GLN:NE2[1_655]	1.64	0.56
1:E:137:ARG:CD	1:F:450:GLU:CG[1_455]	1.64	0.56
1:G:320:LYS:CE	1:H:457:GLU:OE2[1_455]	1.71	0.49
1:A:195:ARG:O	1:F:493:ARG:NH1[1_456]	1.73	0.47

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	359/443 (81%)	326 (91%)	23 (6%)	10 (3%)	6	37
1	B	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	10	48
1	C	358/443 (81%)	326 (91%)	21 (6%)	11 (3%)	5	34
1	D	372/443 (84%)	334 (90%)	31 (8%)	7 (2%)	10	48
1	E	358/443 (81%)	327 (91%)	21 (6%)	10 (3%)	6	37
1	F	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	10	48
1	G	359/443 (81%)	328 (91%)	21 (6%)	10 (3%)	6	37
1	H	372/443 (84%)	335 (90%)	30 (8%)	7 (2%)	10	48
All	All	2922/3544 (82%)	2650 (91%)	203 (7%)	69 (2%)	7	41

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	A	390	TYR
1	A	433	GLN
1	B	134	ASP
1	B	433	GLN

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	333/395 (84%)	303 (91%)	30 (9%)	12	42
1	B	344/395 (87%)	311 (90%)	33 (10%)	10	38
1	C	333/395 (84%)	302 (91%)	31 (9%)	11	40
1	D	344/395 (87%)	312 (91%)	32 (9%)	11	40
1	E	333/395 (84%)	303 (91%)	30 (9%)	12	42
1	F	344/395 (87%)	312 (91%)	32 (9%)	11	40
1	G	333/395 (84%)	302 (91%)	31 (9%)	11	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	344/395 (87%)	312 (91%)	32 (9%)	11	40
All	All	2708/3160 (86%)	2457 (91%)	251 (9%)	11	40

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	444	LYS
1	E	406	ARG
1	H	364	ILE
1	D	460	LEU
1	E	101	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	196	ASN
1	E	196	ASN
1	H	112	ASN
1	D	269	ASN
1	E	100	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	369/443 (83%)	0.67	36 (9%) 10 7	118, 136, 157, 175	0
1	B	382/443 (86%)	0.61	40 (10%) 8 6	115, 136, 154, 182	0
1	C	368/443 (83%)	0.58	32 (8%) 13 8	119, 134, 158, 178	0
1	D	382/443 (86%)	0.74	56 (14%) 3 2	118, 136, 154, 182	0
1	E	368/443 (83%)	1.18	79 (21%) 1 1	118, 136, 157, 180	0
1	F	382/443 (86%)	1.10	92 (24%) 1 1	118, 137, 153, 182	0
1	G	369/443 (83%)	0.98	55 (14%) 3 2	115, 137, 156, 178	0
1	H	382/443 (86%)	0.95	66 (17%) 2 1	119, 136, 153, 181	0
All	All	3002/3544 (84%)	0.85	456 (15%) 3 2	115, 136, 156, 182	0

The worst 5 of 456 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	PRO	9.9
1	A	434	VAL	9.8
1	G	434	VAL	9.0
1	E	432	THR	8.6
1	E	241	LYS	7.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.