



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:52 PM GMT

PDB ID : 4G3D  
Title : Crystal structure of human NF-kappaB inducing kinase (NIK)  
Authors : Hymowitz, S.G.; de Leon-Boenig G.  
Deposited on : 2012-07-13  
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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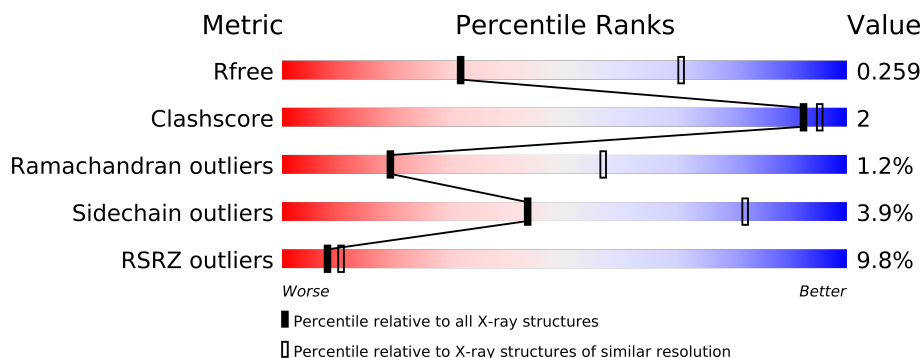
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	371	
1	B	371	
1	D	371	
1	E	371	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	701	-	X
2	MG	D	701	-	X
2	MG	E	701	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9346 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NF-kappa-beta-inducingkinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2493	1572	440	463	18			
1	B	318	Total	C	N	O	S	0	0	0
			2443	1540	433	452	18			
1	D	290	Total	C	N	O	S	0	0	0
			2228	1401	399	410	18			
1	E	283	Total	C	N	O	S	0	0	0
			2161	1354	387	403	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	GLY	-	EXPRESSION TAG	UNP Q99558
A	307	SER	-	EXPRESSION TAG	UNP Q99558
A	674	GLY	-	EXPRESSION TAG	UNP Q99558
A	675	ASN	-	EXPRESSION TAG	UNP Q99558
A	676	SER	-	EXPRESSION TAG	UNP Q99558
B	306	GLY	-	EXPRESSION TAG	UNP Q99558
B	307	SER	-	EXPRESSION TAG	UNP Q99558
B	674	GLY	-	EXPRESSION TAG	UNP Q99558
B	675	ASN	-	EXPRESSION TAG	UNP Q99558
B	676	SER	-	EXPRESSION TAG	UNP Q99558
D	306	GLY	-	EXPRESSION TAG	UNP Q99558
D	307	SER	-	EXPRESSION TAG	UNP Q99558
D	674	GLY	-	EXPRESSION TAG	UNP Q99558
D	675	ASN	-	EXPRESSION TAG	UNP Q99558
D	676	SER	-	EXPRESSION TAG	UNP Q99558
E	306	GLY	-	EXPRESSION TAG	UNP Q99558
E	307	SER	-	EXPRESSION TAG	UNP Q99558
E	674	GLY	-	EXPRESSION TAG	UNP Q99558
E	675	ASN	-	EXPRESSION TAG	UNP Q99558
E	676	SER	-	EXPRESSION TAG	UNP Q99558

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

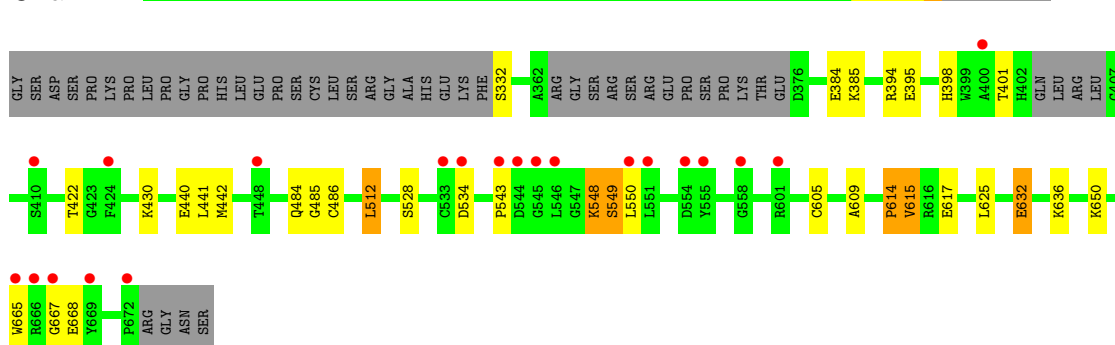
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total 9	O 9	0	0
3	B	8	Total 8	O 8	0	0
3	E	1	Total 1	O 1	0	0

### 3 Residue-property plots

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.

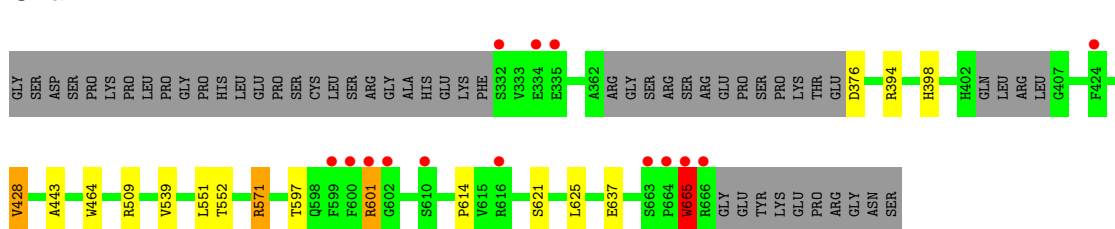
- Molecule 1: NF-kappa-beta-inducingkinase

Chain A:



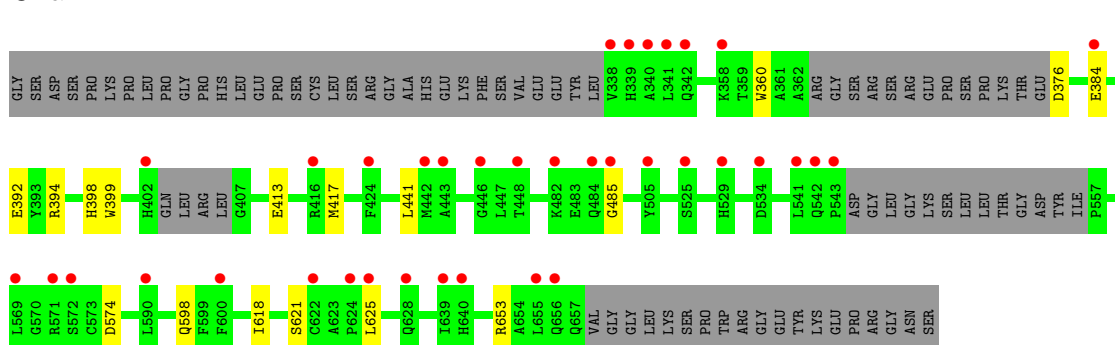
- Molecule 1: NF-kappa-beta-inducingkinase

Chain B:



- Molecule 1: NF-kappa-beta-inducingkinase

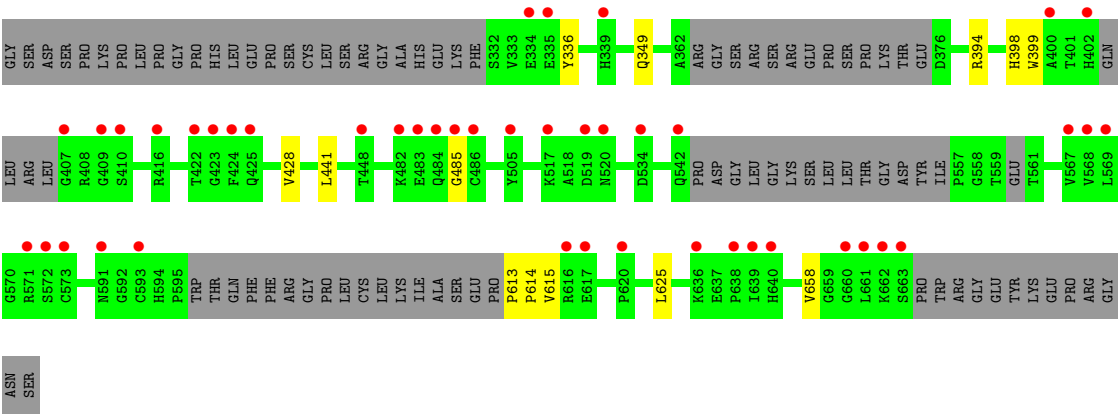
Chain D:



- Molecule 1: NF-kappa-beta-inducingkinase

Chain E:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.75Å 145.85Å 230.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.90 29.68 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.57-2.90) 95.3 (29.68-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.55 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.201 , 0.266 0.196 , 0.259	Depositor DCC
$R_{free}$ test set	2687 reflections (8.66%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 33718 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.51	1/2550 (0.0%)	0.57	1/3453 (0.0%)
1	B	0.51	2/2498 (0.1%)	0.57	1/3383 (0.0%)
1	D	0.49	2/2277 (0.1%)	0.53	0/3081
1	E	0.47	1/2202 (0.0%)	0.50	0/2972
All	All	0.49	6/9527 (0.1%)	0.55	2/12889 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	665	TRP	CD2-CE2	5.28	1.47	1.41
1	D	360	TRP	CD2-CE2	5.21	1.47	1.41
1	B	665	TRP	CD2-CE2	5.17	1.47	1.41
1	D	399	TRP	CD2-CE2	5.14	1.47	1.41
1	B	464	TRP	CD2-CE2	5.10	1.47	1.41
1	E	399	TRP	CD2-CE2	5.02	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	428	VAL	CB-CA-C	-5.01	101.89	111.40



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	443	ALA	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2493	0	7	9	0
1	B	2443	0	0	4	0
1	D	2228	0	0	3	0
1	E	2161	0	0	2	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	9	0	0	0	0
3	B	8	0	0	0	0
3	E	1	0	0	0	0
All	All	9346	0	7	17	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (17) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:484:GLN:O	1:A:486:CYS:N	2.32	0.62
1:A:385:LYS:O	1:A:422:THR:CG2	2.49	0.61
1:A:548:LYS:O	1:A:549:SER:CB	2.50	0.58
1:A:442:MET:O	1:B:601:ARG:NH2	2.42	0.52
1:D:394:ARG:N	1:D:398:HIS:CD2	2.79	0.51
1:A:609:ALA:O	1:A:636:LYS:NZ	2.44	0.51
1:E:394:ARG:N	1:E:398:HIS:CD2	2.81	0.49
1:B:665:TRP:O	1:B:665:TRP:CE3	2.68	0.46
1:A:395:GLU:OE2	1:A:430:LYS:NZ	2.48	0.46
1:A:632:GLU:OE1	1:A:650:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:571:ARG:NH1	1:B:637:GLU:OE2	2.49	0.46
1:D:574:ASP:N	1:D:574:ASP:OD2	2.49	0.44
1:A:394:ARG:N	1:A:398:HIS:CD2	2.87	0.42
1:D:392:GLU:OE1	1:D:394:ARG:NH1	2.52	0.42
1:A:614:PRO:O	1:A:617:GLU:N	2.53	0.42
1:B:394:ARG:N	1:B:398:HIS:CD2	2.88	0.42
1:E:613:PRO:O	1:E:615:VAL:N	2.54	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	318/371 (86%)	295 (93%)	15 (5%)	8 (2%)	9	32
1	B	312/371 (84%)	291 (93%)	19 (6%)	2 (1%)	33	76
1	D	282/371 (76%)	263 (93%)	18 (6%)	1 (0%)	43	82
1	E	271/371 (73%)	256 (94%)	12 (4%)	3 (1%)	21	60
All	All	1183/1484 (80%)	1105 (93%)	64 (5%)	14 (1%)	19	57

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	GLY
1	A	549	SER
1	B	597	THR
1	D	485	GLY
1	A	543	PRO
1	A	548	LYS
1	A	615	VAL
1	A	534	ASP
1	E	658	VAL
1	A	667	GLY
1	E	485	GLY

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Mol	Chain	Res	Type
1	B	614	PRO
1	E	614	PRO
1	A	614	PRO

### 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	266/307 (87%)	253 (95%)	13 (5%)	35	73
1	B	261/307 (85%)	250 (96%)	11 (4%)	40	79
1	D	238/307 (78%)	228 (96%)	10 (4%)	40	79
1	E	231/307 (75%)	226 (98%)	5 (2%)	64	92
All	All	996/1228 (81%)	957 (96%)	39 (4%)	43	82

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	SER
1	A	384	GLU
1	A	401	THR
1	A	440	GLU
1	A	441	LEU
1	A	512	LEU
1	A	528	SER
1	A	550	LEU
1	A	605	CYS
1	A	615	VAL
1	A	625	LEU
1	A	632	GLU
1	A	668	GLU
1	B	376	ASP
1	B	428	VAL
1	B	509	ARG
1	B	539	VAL
1	B	551	LEU
1	B	552	THR

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Mol	Chain	Res	Type
1	B	571	ARG
1	B	601	ARG
1	B	621	SER
1	B	625	LEU
1	B	665	TRP
1	D	376	ASP
1	D	384	GLU
1	D	413	GLU
1	D	417	MET
1	D	441	LEU
1	D	598	GLN
1	D	618	ILE
1	D	621	SER
1	D	625	LEU
1	D	653	ARG
1	E	336	TYR
1	E	349	GLN
1	E	428	VAL
1	E	441	LEU
1	E	625	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 3 ligands modelled in this entry, 3 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.

## 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, 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	324/371 (87%)	0.11	21 (6%) 18 22	35, 55, 113, 186	0
1	B	318/371 (85%)	-0.05	14 (4%) 33 40	34, 55, 117, 188	0
1	D	290/371 (78%)	0.54	37 (12%) 4 6	53, 93, 144, 173	0
1	E	283/371 (76%)	0.72	44 (15%) 3 4	47, 102, 154, 195	0
All	All	1215/1484 (81%)	0.31	116 (9%) 8 11	34, 72, 144, 195	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	543	PRO	12.9
1	E	335	GLU	6.8
1	E	571	ARG	6.8
1	A	543	PRO	6.5
1	D	339	HIS	6.3
1	E	485	GLY	6.1
1	E	572	SER	5.9
1	E	640	HIS	5.9
1	D	442	MET	5.8
1	A	667	GLY	5.8
1	E	663	SER	5.4
1	B	600	PHE	5.1
1	E	639	ILE	4.9
1	E	616	ARG	4.8
1	E	660	GLY	4.6
1	E	424	PHE	4.4
1	E	486	CYS	4.4
1	E	407	GLY	4.2
1	E	569	LEU	4.2
1	E	593	CYS	4.2
1	E	573	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	424	PHE	4.1
1	A	546	LEU	3.7
1	D	446	GLY	3.7
1	D	542	GLN	3.7
1	E	567	VAL	3.7
1	D	402	HIS	3.6
1	D	525	SER	3.6
1	D	384	GLU	3.6
1	D	624	PRO	3.6
1	E	617	GLU	3.5
1	E	484	GLN	3.5
1	A	534	ASP	3.5
1	A	666	ARG	3.5
1	B	665	TRP	3.5
1	B	601	ARG	3.4
1	E	568	VAL	3.4
1	E	662	LYS	3.4
1	E	591	ASN	3.4
1	B	424	PHE	3.3
1	A	665	TRP	3.3
1	D	485	GLY	3.3
1	E	483	GLU	3.2
1	A	544	ASP	3.2
1	D	639	ILE	3.2
1	E	542	GLN	3.2
1	D	342	GLN	3.1
1	A	554	ASP	3.1
1	B	666	ARG	3.1
1	D	640	HIS	3.1
1	E	423	GLY	3.1
1	A	551	LEU	3.1
1	E	402	HIS	3.1
1	A	550	LEU	3.1
1	E	448	THR	3.1
1	B	332	SER	3.0
1	D	534	ASP	3.0
1	E	661	LEU	3.0
1	E	339	HIS	3.0
1	D	572	SER	3.0
1	D	443	ALA	3.0
1	E	636	LYS	3.0
1	E	425	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	334	GLU	2.9
1	E	638	PRO	2.9
1	E	409	GLY	2.9
1	D	571	ARG	2.9
1	A	410	SER	2.9
1	B	334	GLU	2.8
1	E	519	ASP	2.8
1	D	338	VAL	2.8
1	E	505	TYR	2.8
1	B	599	PHE	2.8
1	D	341	LEU	2.7
1	E	400	ALA	2.7
1	D	484	GLN	2.6
1	E	482	LYS	2.6
1	D	529	HIS	2.6
1	D	358	LYS	2.6
1	E	416	ARG	2.5
1	A	558	GLY	2.5
1	D	541	LEU	2.5
1	B	664	PRO	2.5
1	A	448	THR	2.5
1	B	602	GLY	2.5
1	A	424	PHE	2.4
1	B	610	SER	2.4
1	E	517	LYS	2.4
1	B	616	ARG	2.4
1	D	448	THR	2.4
1	A	672	PRO	2.4
1	A	533	CYS	2.3
1	D	655	LEU	2.3
1	D	622	CYS	2.3
1	B	335	GLU	2.3
1	A	555	TYR	2.3
1	D	656	GLN	2.3
1	D	505	TYR	2.3
1	D	628	GLN	2.2
1	E	620	PRO	2.2
1	E	410	SER	2.2
1	A	601	ARG	2.2
1	E	422	THR	2.2
1	E	534	ASP	2.2
1	A	400	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	520	ASN	2.2
1	D	600	PHE	2.1
1	D	569	LEU	2.1
1	D	590	LEU	2.1
1	D	482	LYS	2.1
1	D	340	ALA	2.1
1	A	545	GLY	2.1
1	A	669	TYR	2.1
1	B	663	SER	2.1
1	D	625	LEU	2.1
1	D	416	ARG	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 ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	E	701	1/1	1.46	25.42	81,81,81,81	0
2	MG	D	701	1/1	1.63	19.01	90,90,90,90	0
2	MG	A	701	1/1	1.41	13.99	76,76,76,76	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.