



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:46 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 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

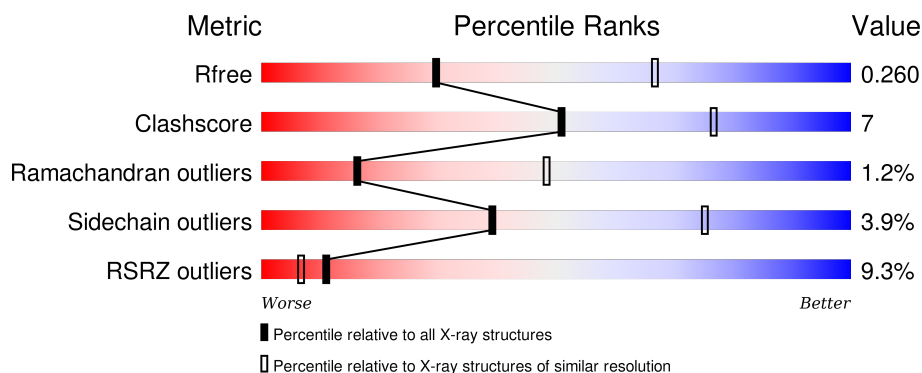
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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  $\geq 3$ , 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	371	<div> <div>3%</div> <div>66%</div> <div>19%</div> <div>••</div> <div>13%</div> </div>
1	B	371	<div> <div>4%</div> <div>68%</div> <div>16%</div> <div>••</div> <div>14%</div> </div>
1	D	371	<div> <div>11%</div> <div>67%</div> <div>11%</div> <div>•</div> <div>22%</div> </div>
1	E	371	<div> <div>12%</div> <div>64%</div> <div>11%</div> <div>•</div> <div>24%</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	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 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 NF-kappa-beta-inducing kinase.

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	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

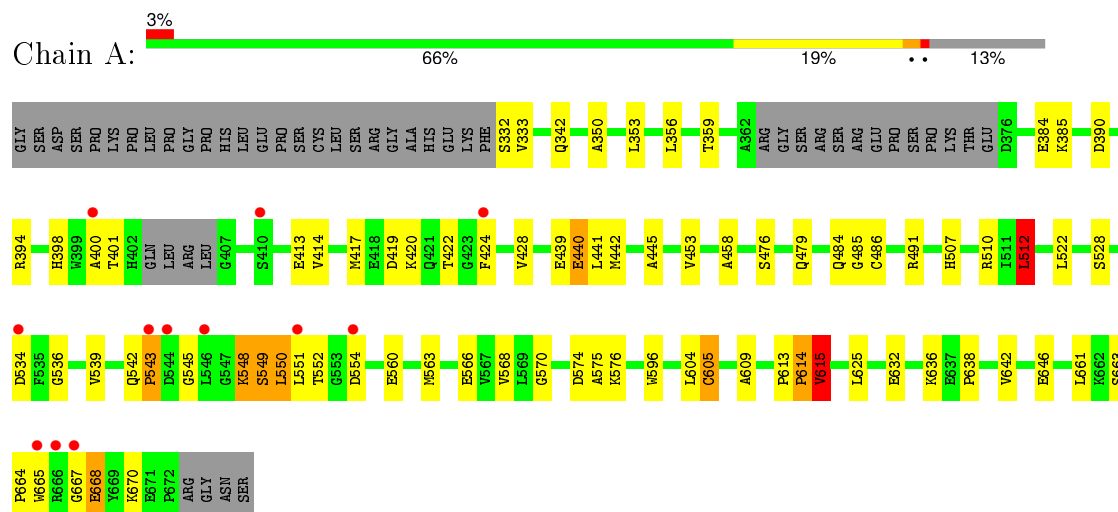
- Molecule 3 is water.

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

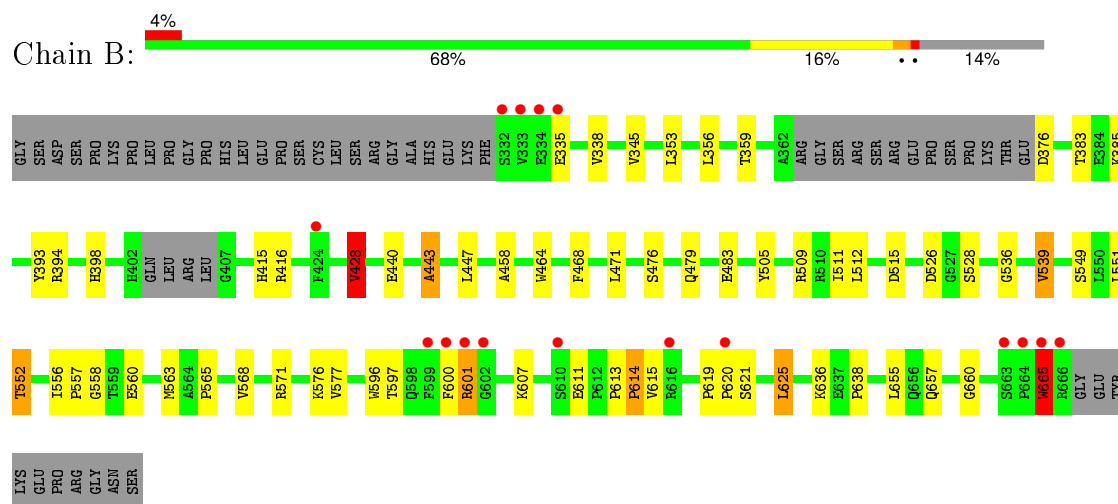
### 3 Residue-property plots

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-inducing kinase

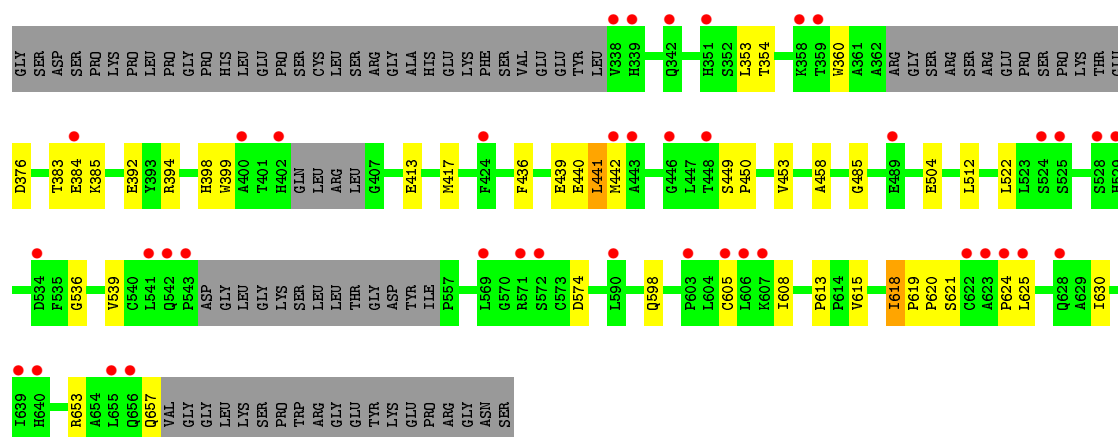


#### • Molecule 1: NF-kappa-beta-inducing kinase

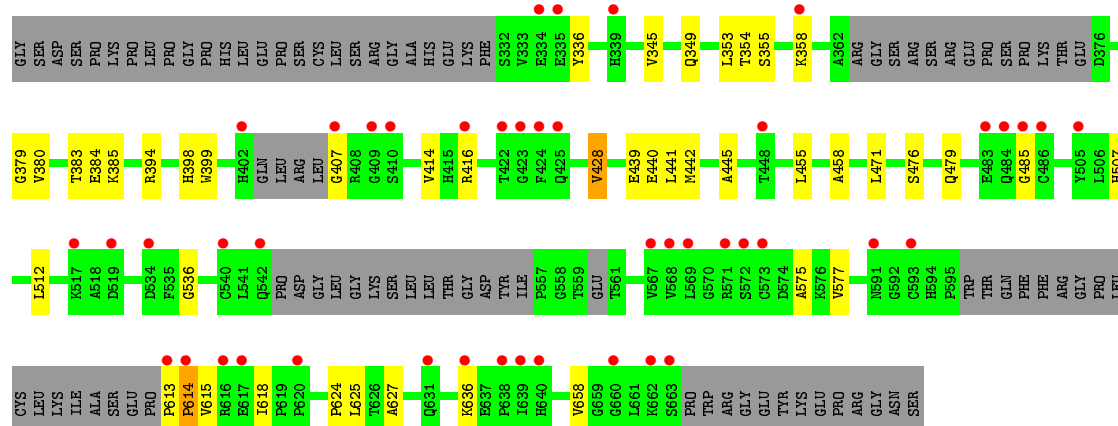


#### • Molecule 1: NF-kappa-beta-inducing kinase





● Molecule 1: NF-kappa-beta-inducing kinase



## 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) 95.4 (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 , 0.260	Depositor DCC
$R_{free}$ test set	2810 reflections (9.06%)	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> )	0.36 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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.

<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

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 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	2493	0	2459	44	0
1	B	2443	0	2415	39	0
1	D	2228	0	2200	22	0
1	E	2161	0	2136	26	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	9210	127	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 7.

All (127) 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:385:LYS:O	1:A:422:THR:HG21	1.55	1.04
1:D:394:ARG:H	1:D:398:HIS:HD2	1.02	1.01
1:E:394:ARG:H	1:E:398:HIS:HD2	1.06	1.00
1:B:394:ARG:H	1:B:398:HIS:HD2	1.12	0.93
1:A:394:ARG:H	1:A:398:HIS:HD2	1.13	0.90
1:E:394:ARG:H	1:E:398:HIS:CD2	1.96	0.83
1:D:394:ARG:H	1:D:398:HIS:CD2	1.94	0.83
1:E:512:LEU:HD11	1:E:577:VAL:HG22	1.66	0.78
1:A:394:ARG:H	1:A:398:HIS:CD2	2.02	0.73
1:B:479:GLN:O	1:B:483:GLU:HG2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLU:HA	1:A:563:MET:HE3	1.71	0.71
1:A:419:ASP:HB3	1:A:422:THR:HG22	1.73	0.70
1:E:383:THR:OG1	1:E:385:LYS:HG2	1.92	0.69
1:B:394:ARG:H	1:B:398:HIS:CD2	2.03	0.67
1:A:548:LYS:O	1:A:549:SER:HB3	1.93	0.67
1:A:642:VAL:HB	1:A:646:GLU:HB3	1.80	0.63
1:A:484:GLN:O	1:A:486:CYS:N	2.32	0.62
1:A:440:GLU:HG2	1:A:536:GLY:HA2	1.81	0.62
1:A:548:LYS:HB3	1:A:554:ASP:HB2	1.80	0.62
1:D:504:GLU:HG2	1:E:624:PRO:HG2	1.81	0.61
1:B:625:LEU:HB2	1:B:657:GLN:OE1	2.01	0.61
1:A:551:LEU:HD12	1:A:570:GLY:HA3	1.83	0.59
1:B:560:GLU:HA	1:B:563:MET:CE	2.32	0.59
1:D:605:CYS:HA	1:D:608:ILE:HD12	1.83	0.59
1:A:439:GLU:HA	1:A:442:MET:HB2	1.83	0.59
1:A:356:LEU:O	1:A:359:THR:HB	2.03	0.59
1:A:568:VAL:HG11	1:A:605:CYS:O	2.03	0.58
1:A:548:LYS:O	1:A:549:SER:CB	2.50	0.58
1:A:422:THR:HG23	1:A:424:PHE:H	1.68	0.58
1:E:353:LEU:HD11	1:E:458:ALA:HB3	1.86	0.58
1:B:440:GLU:HG2	1:B:536:GLY:HA2	1.85	0.57
1:B:476:SER:H	1:B:479:GLN:NE2	2.02	0.57
1:D:394:ARG:N	1:D:398:HIS:HD2	1.87	0.56
1:B:512:LEU:HD21	1:B:577:VAL:HG21	1.88	0.56
1:D:353:LEU:HD11	1:D:458:ALA:HB3	1.88	0.55
1:A:510:ARG:HH12	1:A:545:GLY:H	1.53	0.55
1:A:548:LYS:HD2	1:A:554:ASP:HB3	1.88	0.55
1:B:549:SER:H	1:B:552:THR:HG22	1.73	0.54
1:D:440:GLU:HG2	1:D:536:GLY:HA2	1.90	0.54
1:A:453:VAL:HG21	1:A:522:LEU:HD12	1.88	0.54
1:E:354:THR:HG23	1:E:442:MET:HG2	1.90	0.53
1:E:416:ARG:HE	1:E:471:LEU:HD21	1.74	0.53
1:A:353:LEU:HD11	1:A:458:ALA:HB3	1.89	0.53
1:B:512:LEU:HB3	1:B:539:VAL:HG22	1.90	0.52
1:A:566:GLU:CD	1:A:638:PRO:HG3	2.30	0.52
1:D:512:LEU:HD22	1:D:539:VAL:HG22	1.91	0.52
1:A:442:MET:O	1:B:601:ARG:NH2	2.42	0.52
1:A:574:ASP:OD2	1:A:576:LYS:HB2	2.09	0.52
1:B:353:LEU:HD11	1:B:458:ALA:HB3	1.92	0.51
1:A:342:GLN:HE21	1:A:359:THR:HG21	1.75	0.51
1:A:390:ASP:OD2	1:B:415:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ALA:O	1:A:636:LYS:NZ	2.44	0.51
1:A:512:LEU:HD22	1:A:539:VAL:HG22	1.92	0.50
1:A:507:HIS:CG	1:A:575:ALA:HB1	2.45	0.50
1:A:333:VAL:HG11	1:B:568:VAL:HG23	1.94	0.50
1:E:613:PRO:HG3	1:E:636:LYS:HG3	1.93	0.50
1:E:394:ARG:N	1:E:398:HIS:HD2	1.91	0.50
1:A:417:MET:HB3	1:A:428:VAL:CG2	2.42	0.50
1:A:413:GLU:HG3	1:A:414:VAL:HG23	1.94	0.50
1:D:354:THR:HG23	1:D:442:MET:HG2	1.93	0.49
1:B:440:GLU:CG	1:B:536:GLY:HA2	2.43	0.49
1:A:596:TRP:CZ2	1:A:614:PRO:HG3	2.48	0.49
1:B:515:ASP:CG	1:B:558:GLY:HA3	2.33	0.49
1:E:613:PRO:C	1:E:615:VAL:H	2.15	0.49
1:E:414:VAL:HA	1:E:428:VAL:O	2.13	0.49
1:D:613:PRO:HB2	1:D:615:VAL:HG23	1.94	0.49
1:E:439:GLU:HA	1:E:442:MET:HB2	1.93	0.48
1:A:550:LEU:HD23	1:A:551:LEU:HG	1.94	0.48
1:D:439:GLU:HA	1:D:442:MET:HB2	1.96	0.48
1:A:542:GLN:HB2	1:A:543:PRO:HD2	1.95	0.48
1:B:556:ILE:HG13	1:B:557:PRO:HD2	1.96	0.48
1:B:613:PRO:HG3	1:B:636:LYS:HG3	1.95	0.48
1:A:440:GLU:CG	1:A:536:GLY:HA2	2.42	0.48
1:B:335:GLU:HA	1:B:338:VAL:HG22	1.96	0.48
1:E:355:SER:HA	1:E:358:LYS:HD2	1.96	0.47
1:E:445:ALA:HA	1:E:455:LEU:HD23	1.96	0.47
1:D:624:PRO:HD2	1:D:657:GLN:HE22	1.80	0.47
1:A:549:SER:O	1:A:552:THR:HG22	2.15	0.47
1:B:560:GLU:HA	1:B:563:MET:HE3	1.95	0.47
1:B:416:ARG:HE	1:B:471:LEU:HD21	1.80	0.47
1:E:613:PRO:HD3	1:E:636:LYS:HD2	1.97	0.47
1:A:400:ALA:HB2	1:A:420:LYS:HE3	1.97	0.46
1:B:665:TRP:CE3	1:B:665:TRP:O	2.68	0.46
1:E:353:LEU:HD13	1:E:380:VAL:HB	1.98	0.46
1:B:576:LYS:HG2	1:B:638:PRO:O	2.16	0.46
1:D:615:VAL:O	1:D:618:ILE:HB	2.16	0.46
1:E:618:ILE:HD11	1:E:627:ALA:HA	1.97	0.45
1:D:618:ILE:HD11	1:D:630:ILE:HB	1.98	0.45
1:B:596:TRP:CZ2	1:B:614:PRO:HG3	2.52	0.45
1:D:453:VAL:HG21	1:D:522:LEU:HD12	1.99	0.45
1:B:345:VAL:HG11	1:B:393:TYR:HB2	1.99	0.45
1:B:613:PRO:C	1:B:615:VAL:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:PRO:HA	1:B:620:PRO:HD3	1.88	0.44
1:D:574:ASP:N	1:D:574:ASP:OD2	2.49	0.44
1:A:476:SER:H	1:A:479:GLN:NE2	2.16	0.44
1:A:491:ARG:HD2	1:A:661:LEU:HD11	2.00	0.44
1:B:512:LEU:HD21	1:B:577:VAL:CG2	2.47	0.43
1:A:613:PRO:C	1:A:615:VAL:H	2.22	0.43
1:E:507:HIS:CG	1:E:575:ALA:HB1	2.54	0.43
1:E:407:GLY:HA2	1:E:414:VAL:O	2.18	0.43
1:A:350:ALA:HB1	1:A:445:ALA:HB1	2.01	0.43
1:E:440:GLU:HG2	1:E:536:GLY:HA2	2.00	0.43
1:E:384:GLU:H	1:E:384:GLU:CD	2.22	0.43
1:B:565:PRO:O	1:B:568:VAL:HG12	2.18	0.43
1:E:613:PRO:HA	1:E:614:PRO:HD3	1.94	0.43
1:B:428:VAL:HG13	1:B:468:PHE:CE2	2.54	0.42
1:D:392:GLU:OE1	1:D:394:ARG:NH1	2.52	0.42
1:E:613:PRO:HB2	1:E:615:VAL:HG23	2.02	0.42
1:B:607:LYS:HD2	1:B:611:GLU:HG2	2.01	0.42
1:B:526:ASP:OD1	1:B:528:SER:HB3	2.20	0.42
1:B:383:THR:OG1	1:B:385:LYS:HG2	2.20	0.41
1:A:668:GLU:HG3	1:A:670:LYS:HE2	2.03	0.41
1:D:449:SER:HA	1:D:450:PRO:HD3	1.94	0.41
1:D:436:PHE:HZ	1:D:441:LEU:CD2	2.33	0.41
1:D:383:THR:OG1	1:D:385:LYS:HG2	2.20	0.41
1:D:613:PRO:C	1:D:615:VAL:H	2.24	0.41
1:D:619:PRO:HA	1:D:620:PRO:HD3	1.89	0.41
1:E:345:VAL:HA	1:E:379:GLY:O	2.21	0.41
1:B:596:TRP:HE3	1:B:600:PHE:CZ	2.38	0.41
1:B:447:LEU:HB3	1:B:505:TYR:HE1	1.86	0.41
1:B:356:LEU:O	1:B:359:THR:HB	2.21	0.41
1:B:443:ALA:HA	1:B:511:ILE:HD13	2.03	0.41
1:A:663:SER:HA	1:A:664:PRO:HD3	1.98	0.41
1:E:476:SER:H	1:E:479:GLN:NE2	2.20	0.40
1:B:655:LEU:HD23	1:B:660:GLY:HA2	2.03	0.40
1:B:560:GLU:HA	1:B:563:MET:HE2	2.01	0.40
1:A:596:TRP:HB3	1:A:604:LEU:HD22	2.03	0.40

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	318/371 (86%)	295 (93%)	15 (5%)	8 (2%)	7	27
1	B	312/371 (84%)	291 (93%)	19 (6%)	2 (1%)	30	67
1	D	282/371 (76%)	263 (93%)	18 (6%)	1 (0%)	39	74
1	E	271/371 (73%)	256 (94%)	12 (4%)	3 (1%)	17	51
All	All	1183/1484 (80%)	1105 (93%)	64 (5%)	14 (1%)	16	48

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
1	B	614	PRO
1	E	614	PRO
1	A	614	PRO

### 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	266/307 (87%)	253 (95%)	13 (5%)	31	67
1	B	261/307 (85%)	250 (96%)	11 (4%)	36	73
1	D	238/307 (78%)	228 (96%)	10 (4%)	36	73
1	E	231/307 (75%)	226 (98%)	5 (2%)	60	88
All	All	996/1228 (81%)	957 (96%)	39 (4%)	39	75

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
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

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Mol	Chain	Res	Type
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. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	GLN
1	A	398	HIS
1	A	425	GLN
1	A	484	GLN
1	A	598	GLN
1	A	628	GLN
1	B	398	HIS
1	B	415	HIS
1	B	425	GLN
1	B	479	GLN
1	D	398	HIS
1	D	657	GLN
1	E	398	HIS
1	E	425	GLN
1	E	479	GLN
1	E	507	HIS
1	E	562	HIS
1	E	628	GLN

### 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

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.

No monomer is involved in short contacts.

## 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%)	0.06	12 (3%) 45 38	35, 55, 113, 186	0
1	B	318/371 (85%)	-0.03	16 (5%) 32 26	34, 55, 117, 188	0
1	D	290/371 (78%)	0.63	40 (13%) 4 2	53, 93, 144, 173	0
1	E	283/371 (76%)	0.65	45 (15%) 3 1	47, 102, 154, 195	0
All	All	1215/1484 (81%)	0.31	113 (9%) 11 7	34, 72, 144, 195	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	543	PRO	9.7
1	E	335	GLU	7.1
1	D	339	HIS	6.9
1	A	543	PRO	6.7
1	D	442	MET	6.5
1	A	667	GLY	5.9
1	E	663	SER	5.8
1	E	571	ARG	5.8
1	E	616	ARG	5.5
1	E	640	HIS	5.5
1	B	600	PHE	5.1
1	B	332	SER	4.9
1	E	572	SER	4.8
1	D	624	PRO	4.8
1	E	617	GLU	4.7
1	B	334	GLU	4.6
1	E	485	GLY	4.4
1	A	546	LEU	4.2
1	D	525	SER	3.9
1	E	593	CYS	3.9
1	E	639	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	407	GLY	3.8
1	A	544	ASP	3.7
1	B	665	TRP	3.7
1	D	424	PHE	3.7
1	B	601	ARG	3.5
1	D	358	LYS	3.5
1	D	446	GLY	3.5
1	D	542	GLN	3.4
1	D	628	GLN	3.4
1	E	660	GLY	3.4
1	D	529	HIS	3.4
1	D	402	HIS	3.4
1	E	424	PHE	3.4
1	D	622	CYS	3.4
1	E	591	ASN	3.4
1	E	409	GLY	3.4
1	D	384	GLU	3.4
1	E	542	GLN	3.4
1	E	448	THR	3.3
1	E	569	LEU	3.3
1	D	572	SER	3.2
1	E	614	PRO	3.2
1	E	567	VAL	3.2
1	E	410	SER	3.2
1	A	554	ASP	3.2
1	E	568	VAL	3.1
1	E	339	HIS	3.1
1	B	335	GLU	3.1
1	E	486	CYS	3.1
1	D	625	LEU	3.1
1	E	402	HIS	3.1
1	A	665	TRP	3.1
1	B	610	SER	3.0
1	E	573	CYS	3.0
1	B	424	PHE	3.0
1	E	425	GLN	3.0
1	B	666	ARG	2.9
1	D	338	VAL	2.9
1	E	636	LYS	2.9
1	E	334	GLU	2.9
1	A	424	PHE	2.8
1	D	541	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	606	LEU	2.8
1	D	656	GLN	2.8
1	D	534	ASP	2.8
1	D	351	HIS	2.8
1	E	505	TYR	2.8
1	D	342	GLN	2.8
1	E	613	PRO	2.7
1	D	359	THR	2.7
1	A	666	ARG	2.7
1	E	423	GLY	2.7
1	D	443	ALA	2.6
1	D	655	LEU	2.6
1	D	569	LEU	2.6
1	D	448	THR	2.6
1	D	623	ALA	2.6
1	E	620	PRO	2.6
1	E	519	ASP	2.6
1	E	484	GLN	2.6
1	E	631	GLN	2.6
1	A	534	ASP	2.5
1	E	662	LYS	2.5
1	A	410	SER	2.5
1	D	571	ARG	2.5
1	E	540	CYS	2.5
1	B	664	PRO	2.4
1	D	605	CYS	2.4
1	E	483	GLU	2.4
1	D	400	ALA	2.4
1	E	517	LYS	2.4
1	B	333	VAL	2.4
1	B	602	GLY	2.4
1	D	524	SER	2.4
1	D	528	SER	2.4
1	D	640	HIS	2.3
1	D	607	LYS	2.3
1	B	599	PHE	2.3
1	E	638	PRO	2.3
1	B	616	ARG	2.2
1	A	551	LEU	2.2
1	A	400	ALA	2.2
1	E	534	ASP	2.2
1	D	639	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	590	LEU	2.2
1	E	416	ARG	2.1
1	E	422	THR	2.1
1	B	663	SER	2.1
1	B	620	PRO	2.1
1	D	489	GLU	2.0
1	E	358	LYS	2.0
1	D	603	PRO	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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	D	701	1/1	0.67	1.61	23.55	90,90,90,90	0
2	MG	E	701	1/1	0.82	1.57	20.63	81,81,81,81	0
2	MG	A	701	1/1	0.91	1.33	15.26	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.