



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:22 PM GMT

PDB ID : 4EJQ  
Title : Crystal structure of KIF1A C-CC1-FHA  
Authors : Huo, L.; Yue, Y.; Ren, J.; Yu, J.; Liu, J.; Yu, Y.; Ye, F.; Xu, T.; Zhang, M.;  
Feng, W.  
Deposited on : 2012-04-06  
Resolution : 1.89 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

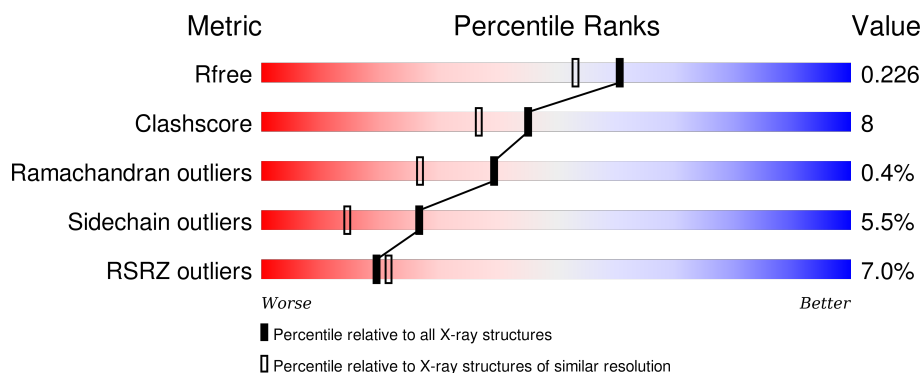
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	154	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	B	154	<div> <div>8%</div> <div>68%</div> <div>21%</div> <div>8%</div> </div>
1	C	154	<div> <div>6%</div> <div>81%</div> <div>16%</div> </div>
1	D	154	<div> <div>5%</div> <div>79%</div> <div>16%</div> </div>
1	E	154	<div> <div>5%</div> <div>82%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	154	<div><div></div><div>8%</div><div>79%</div><div>17%</div><div></div><div></div></div>
1	G	154	<div><div></div><div>14%</div><div>69%</div><div>19%</div><div>6%</div><div>5%</div></div>
1	H	154	<div><div></div><div>4%</div><div>86%</div><div>13%</div><div></div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10054 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 Kinesin-like protein KIF1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1214	747	224	235	8			
1	B	142	Total	C	N	O	S	0	0	0
			1114	693	200	213	8			
1	C	151	Total	C	N	O	S	0	0	0
			1187	732	218	229	8			
1	D	148	Total	C	N	O	S	0	0	0
			1166	721	212	225	8			
1	E	148	Total	C	N	O	S	0	0	0
			1166	721	212	225	8			
1	F	151	Total	C	N	O	S	0	0	0
			1187	732	218	229	8			
1	G	146	Total	C	N	O	S	0	0	0
			1148	711	210	219	8			
1	H	154	Total	C	N	O	S	0	0	0
			1214	747	224	235	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	GLY	-	EXPRESSION TAG	UNP Q12756
A	455	SER	-	EXPRESSION TAG	UNP Q12756
A	456	GLU	-	EXPRESSION TAG	UNP Q12756
A	457	PHE	-	EXPRESSION TAG	UNP Q12756
B	454	GLY	-	EXPRESSION TAG	UNP Q12756
B	455	SER	-	EXPRESSION TAG	UNP Q12756
B	456	GLU	-	EXPRESSION TAG	UNP Q12756
B	457	PHE	-	EXPRESSION TAG	UNP Q12756
C	454	GLY	-	EXPRESSION TAG	UNP Q12756
C	455	SER	-	EXPRESSION TAG	UNP Q12756
C	456	GLU	-	EXPRESSION TAG	UNP Q12756
C	457	PHE	-	EXPRESSION TAG	UNP Q12756
D	454	GLY	-	EXPRESSION TAG	UNP Q12756

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Chain	Residue	Modelled	Actual	Comment	Reference
D	455	SER	-	EXPRESSION TAG	UNP Q12756
D	456	GLU	-	EXPRESSION TAG	UNP Q12756
D	457	PHE	-	EXPRESSION TAG	UNP Q12756
E	454	GLY	-	EXPRESSION TAG	UNP Q12756
E	455	SER	-	EXPRESSION TAG	UNP Q12756
E	456	GLU	-	EXPRESSION TAG	UNP Q12756
E	457	PHE	-	EXPRESSION TAG	UNP Q12756
F	454	GLY	-	EXPRESSION TAG	UNP Q12756
F	455	SER	-	EXPRESSION TAG	UNP Q12756
F	456	GLU	-	EXPRESSION TAG	UNP Q12756
F	457	PHE	-	EXPRESSION TAG	UNP Q12756
G	454	GLY	-	EXPRESSION TAG	UNP Q12756
G	455	SER	-	EXPRESSION TAG	UNP Q12756
G	456	GLU	-	EXPRESSION TAG	UNP Q12756
G	457	PHE	-	EXPRESSION TAG	UNP Q12756
H	454	GLY	-	EXPRESSION TAG	UNP Q12756
H	455	SER	-	EXPRESSION TAG	UNP Q12756
H	456	GLU	-	EXPRESSION TAG	UNP Q12756
H	457	PHE	-	EXPRESSION TAG	UNP Q12756

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	119	Total O 119 119	0	0
2	B	50	Total O 50 50	0	0
2	C	88	Total O 88 88	0	0
2	D	78	Total O 78 78	0	0
2	E	80	Total O 80 80	0	0
2	F	81	Total O 81 81	0	0
2	G	49	Total O 49 49	0	0
2	H	113	Total O 113 113	0	0

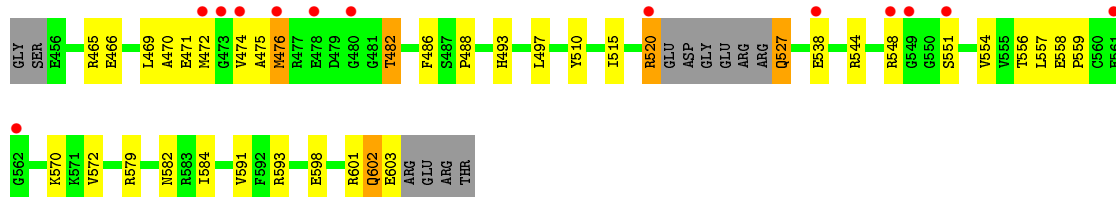
### 3 Residue-property plots [i](#)

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.

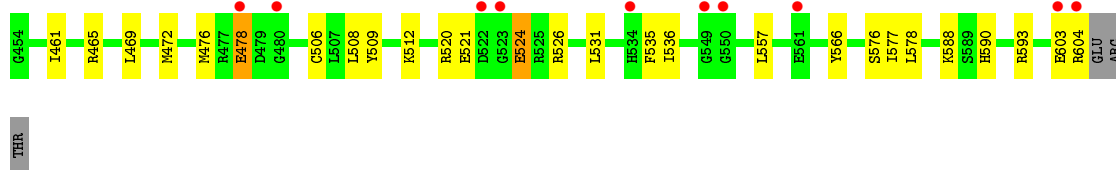
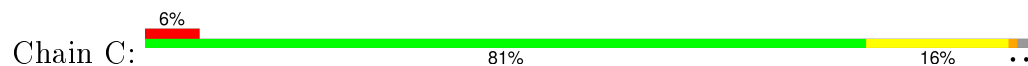
- Molecule 1: Kinesin-like protein KIF1A



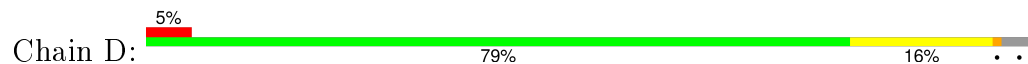
- Molecule 1: Kinesin-like protein KIF1A



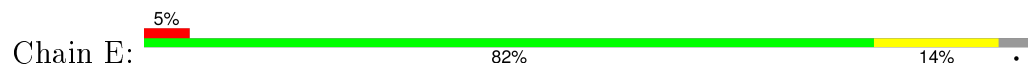
- Molecule 1: Kinesin-like protein KIF1A



- Molecule 1: Kinesin-like protein KIF1A

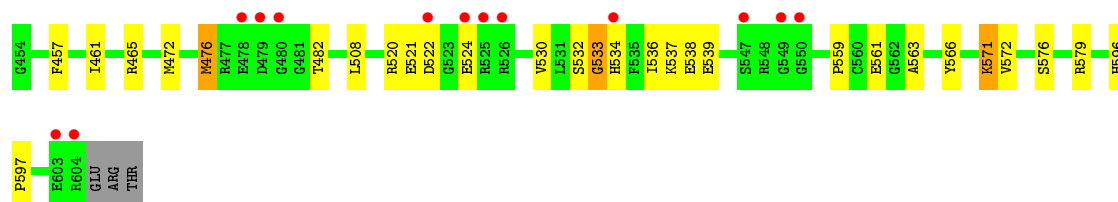
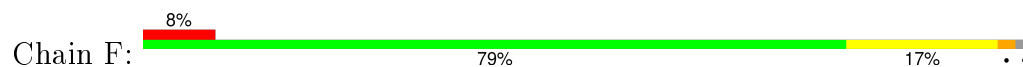


- Molecule 1: Kinesin-like protein KIF1A

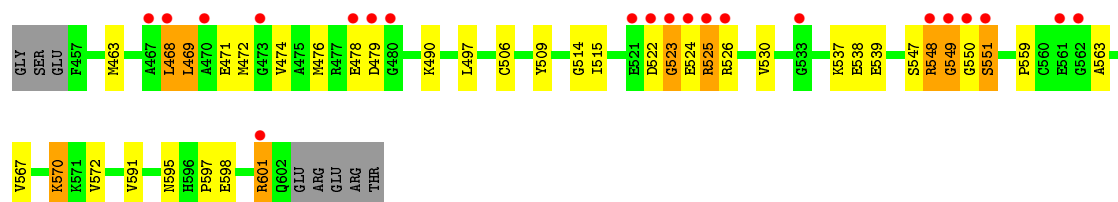




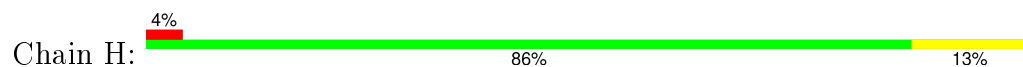
- Molecule 1: Kinesin-like protein KIF1A



- Molecule 1: Kinesin-like protein KIF1A



- Molecule 1: Kinesin-like protein KIF1A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.95Å 57.84Å 110.39Å 89.98° 89.96° 90.63°	Depositor
Resolution (Å)	33.91 – 1.89 33.90 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.0 (33.91-1.89) 94.0 (33.90-1.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.187 , 0.231 0.184 , 0.226	Depositor DCC
$R_{free}$ test set	1957 reflections (2.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.3	EDS
Estimated twinning fraction	0.045 for h,-k,-l 0.048 for -h,k,-l 0.458 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 82040 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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 [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	0.42	0/1233	0.56	0/1654
1	B	0.33	0/1132	0.57	0/1520
1	C	0.35	0/1206	0.54	0/1618
1	D	0.39	0/1185	0.57	0/1591
1	E	0.37	0/1185	0.56	0/1591
1	F	0.35	0/1206	0.53	0/1618
1	G	0.34	0/1167	0.60	1/1567 (0.1%)
1	H	0.43	0/1233	0.61	1/1654 (0.1%)
All	All	0.37	0/9547	0.57	2/12813 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	549	GLY	N-CA-C	-8.90	90.85	113.10
1	H	524	GLU	CB-CA-C	-5.01	100.38	110.40

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	1214	0	1193	8	0
1	B	1114	0	1100	32	0
1	C	1187	0	1167	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1166	0	1146	20	0
1	E	1166	0	1146	16	0
1	F	1187	0	1167	18	0
1	G	1148	0	1134	27	0
1	H	1214	0	1193	19	0
2	A	119	0	0	1	0
2	B	50	0	0	1	0
2	C	88	0	0	3	0
2	D	78	0	0	2	0
2	E	80	0	0	3	0
2	F	81	0	0	2	0
2	G	49	0	0	0	0
2	H	113	0	0	3	0
All	All	10054	0	9246	146	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 8.

All (146) 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:G:471:GLU:HG2	1:G:472:MET:SD	1.76	1.24
1:B:520:ARG:HH11	1:B:520:ARG:HG2	1.13	1.11
1:B:548:ARG:HH21	1:B:554:VAL:HG21	0.92	1.08
1:B:548:ARG:NH2	1:B:554:VAL:HG21	1.74	1.01
1:H:522:ASP:OD2	1:H:526:ARG:HA	1.66	0.94
1:C:536:ILE:HD11	1:C:590:HIS:CD2	2.03	0.93
1:E:521:GLU:HG3	1:E:530:VAL:HG11	1.50	0.90
1:B:548:ARG:HH21	1:B:554:VAL:CG2	1.84	0.87
1:G:478:GLU:HB2	1:H:526:ARG:HH22	1.42	0.85
1:G:471:GLU:CG	1:G:472:MET:SD	2.64	0.85
1:D:477:ARG:HB2	1:D:480:GLY:O	1.82	0.80
1:B:520:ARG:HG2	1:B:520:ARG:NH1	1.91	0.80
1:B:520:ARG:HH11	1:B:520:ARG:CG	1.93	0.78
1:E:556:THR:HG22	1:E:577:ILE:HD13	1.65	0.77
1:F:566:TYR:HE1	1:F:571:LYS:HE2	1.52	0.74
1:B:472:MET:HB3	1:B:474:VAL:HG23	1.70	0.73
1:B:469:LEU:HD13	1:B:476:MET:SD	2.29	0.71
1:C:577:ILE:H	1:C:577:ILE:HD12	1.55	0.71
1:H:521:GLU:HG2	1:H:530:VAL:HG11	1.71	0.71
1:B:527:GLN:HE21	1:B:527:GLN:CA	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:595:ASN:ND2	1:H:501:PRO:HG3	2.08	0.68
1:G:567:VAL:O	1:G:570:LYS:HG3	1.94	0.68
1:F:566:TYR:CE1	1:F:571:LYS:HE2	2.32	0.65
1:H:522:ASP:HB3	1:H:523:GLY:O	1.95	0.65
1:D:477:ARG:C	1:D:480:GLY:H	2.00	0.64
1:B:579:ARG:H	1:B:582:ASN:ND2	1.96	0.64
1:G:478:GLU:HB2	1:H:526:ARG:NH2	2.13	0.63
1:E:469:LEU:HD13	1:E:476:MET:SD	2.38	0.63
1:H:472:MET:HB3	2:H:779:HOH:O	1.98	0.63
1:D:524:GLU:HG2	1:D:525:ARG:N	2.12	0.62
1:H:522:ASP:OD2	1:H:526:ARG:HD2	1.99	0.62
1:C:476:MET:HB3	1:G:551:SER:HB2	1.80	0.62
1:A:474:VAL:HG21	1:B:472:MET:HG2	1.82	0.62
1:D:521:GLU:N	1:D:521:GLU:OE1	2.29	0.61
1:C:524:GLU:CD	1:C:524:GLU:H	2.03	0.61
1:F:521:GLU:HB2	1:F:530:VAL:HG11	1.82	0.61
1:C:535:PHE:CD2	1:C:588:LYS:HG3	2.35	0.61
1:E:547:SER:HB3	2:E:765:HOH:O	2.03	0.59
1:D:477:ARG:O	1:D:480:GLY:N	2.35	0.58
1:D:551:SER:O	2:D:706:HOH:O	2.17	0.58
1:C:520:ARG:HD2	1:C:536:ILE:O	2.04	0.58
1:E:565:THR:O	1:E:572:VAL:HG22	2.04	0.57
1:H:475:ALA:HB2	1:H:486:PHE:CE2	2.39	0.57
1:H:548:ARG:HB3	1:H:548:ARG:HH11	1.69	0.56
1:A:588:LYS:HD3	1:D:534:HIS:HB2	1.88	0.56
1:B:602:GLN:HG2	1:F:465:ARG:NH2	2.21	0.56
1:B:488:PRO:HG3	1:B:510:TYR:HE1	1.71	0.55
1:A:475:ALA:HB2	1:A:486:PHE:CE2	2.43	0.54
1:G:515:ILE:N	1:G:515:ILE:HD12	2.23	0.54
1:C:461:ILE:HD13	1:D:461:ILE:HG12	1.90	0.53
1:G:559:PRO:HD3	1:G:572:VAL:CG1	2.38	0.53
1:G:472:MET:HA	1:G:472:MET:CE	2.38	0.52
1:E:482:THR:HG21	1:F:472:MET:CE	2.39	0.52
1:F:597:PRO:HD2	2:F:712:HOH:O	2.08	0.52
1:B:527:GLN:HE21	1:B:527:GLN:HA	1.72	0.52
1:H:601:ARG:NH1	2:H:788:HOH:O	2.42	0.52
1:F:520:ARG:HD2	1:F:536:ILE:O	2.11	0.51
1:B:527:GLN:NE2	1:B:527:GLN:CA	2.73	0.51
1:C:465:ARG:HD3	2:C:750:HOH:O	2.10	0.51
1:D:475:ALA:HB2	1:D:486:PHE:CE2	2.46	0.51
1:B:527:GLN:NE2	1:B:527:GLN:HA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:469:LEU:HD23	1:G:476:MET:HG3	1.93	0.50
1:D:521:GLU:CD	1:D:521:GLU:H	2.13	0.50
1:B:488:PRO:HD2	1:B:493:HIS:CE1	2.47	0.50
1:B:476:MET:HE1	1:B:482:THR:HG23	1.94	0.49
1:H:472:MET:HE3	2:H:779:HOH:O	2.11	0.49
1:G:598:GLU:O	1:G:601:ARG:HG3	2.12	0.49
1:B:497:LEU:HD12	1:B:591:VAL:HG12	1.93	0.49
1:B:557:LEU:HD22	1:B:584:ILE:HD13	1.95	0.48
1:G:522:ASP:O	1:G:523:GLY:O	2.31	0.48
1:H:547:SER:C	1:H:549:GLY:N	2.67	0.48
1:H:521:GLU:HG2	1:H:530:VAL:CG1	2.42	0.48
1:E:475:ALA:HB2	1:E:486:PHE:CE2	2.48	0.48
1:D:476:MET:HE3	1:D:481:GLY:N	2.28	0.48
1:A:559:PRO:HD3	1:A:572:VAL:HG12	1.96	0.48
1:D:518:VAL:HG22	1:D:529:ILE:HB	1.96	0.48
1:G:472:MET:C	1:G:474:VAL:H	2.18	0.47
1:E:556:THR:CG2	1:E:577:ILE:HD13	2.39	0.47
1:B:598:GLU:HA	1:B:601:ARG:HH11	1.80	0.47
1:D:483:LEU:HD12	2:D:750:HOH:O	2.14	0.47
1:G:524:GLU:HG2	1:G:538:GLU:OE1	2.15	0.47
1:D:477:ARG:O	1:D:480:GLY:CA	2.63	0.47
1:A:588:LYS:NZ	2:A:783:HOH:O	2.48	0.47
1:G:559:PRO:HD3	1:G:572:VAL:HG12	1.97	0.47
1:A:488:PRO:HG3	1:A:510:TYR:HE1	1.80	0.47
1:E:483:LEU:HD12	2:E:762:HOH:O	2.15	0.46
1:G:537:LYS:HG3	1:G:563:ALA:HB2	1.97	0.46
1:F:457:PHE:O	1:F:461:ILE:HG12	2.15	0.46
1:C:531:LEU:HB3	1:C:536:ILE:HD13	1.97	0.46
1:B:476:MET:CE	1:B:482:THR:HG23	2.45	0.46
1:C:566:TYR:HD1	2:C:740:HOH:O	1.98	0.46
1:G:468:LEU:O	1:G:471:GLU:HB3	2.16	0.45
1:E:482:THR:HG21	1:F:472:MET:HE3	1.98	0.45
1:G:525:ARG:HD3	1:G:539:GLU:OE2	2.17	0.45
1:C:472:MET:CE	1:D:482:THR:HG21	2.46	0.45
1:D:557:LEU:HB2	1:D:578:LEU:HD11	1.98	0.45
1:B:544:ARG:HB2	1:B:556:THR:HG22	1.98	0.45
1:F:532:SER:HA	1:F:533:GLY:HA3	1.63	0.45
1:C:593:ARG:HD2	2:C:727:HOH:O	2.17	0.45
1:B:527:GLN:HE21	1:B:527:GLN:N	2.14	0.45
1:C:506:CYS:HB2	1:C:509:TYR:CZ	2.52	0.45
1:E:521:GLU:CG	1:E:530:VAL:HG11	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:PHE:HD2	1:C:588:LYS:HG3	1.82	0.44
1:H:471:GLU:HG2	1:H:472:MET:SD	2.58	0.44
1:F:571:LYS:HB2	1:F:571:LYS:HE3	1.62	0.44
1:C:524:GLU:CD	1:C:524:GLU:N	2.69	0.44
1:A:548:ARG:HA	1:A:549:GLY:HA2	1.47	0.44
1:B:544:ARG:HB2	1:B:556:THR:CG2	2.48	0.44
1:A:464:GLU:O	1:A:468:LEU:HB2	2.18	0.44
1:C:531:LEU:CB	1:C:536:ILE:HD13	2.47	0.43
1:B:559:PRO:HG3	1:B:572:VAL:HB	1.99	0.43
1:G:548:ARG:HB2	1:G:549:GLY:H	1.44	0.43
1:D:469:LEU:HD13	1:D:476:MET:SD	2.58	0.43
1:B:470:ALA:C	1:B:472:MET:H	2.22	0.43
1:F:559:PRO:HD3	1:F:572:VAL:HG12	1.99	0.43
1:G:514:GLY:C	1:G:515:ILE:HD12	2.39	0.42
1:B:593:ARG:NH2	2:B:725:HOH:O	2.50	0.42
1:E:551:SER:HA	2:E:776:HOH:O	2.18	0.42
1:C:536:ILE:HD11	1:C:590:HIS:NE2	2.31	0.42
1:E:524:GLU:H	1:E:524:GLU:CD	2.22	0.42
1:G:597:PRO:O	1:G:601:ARG:HG2	2.19	0.42
1:H:535:PHE:CE2	1:H:588:LYS:HD2	2.54	0.42
1:F:579:ARG:HD2	2:F:756:HOH:O	2.19	0.42
1:D:520:ARG:O	1:D:527:GLN:HG3	2.19	0.42
1:H:535:PHE:CD2	1:H:588:LYS:HD2	2.54	0.42
1:D:524:GLU:CG	1:D:525:ARG:N	2.81	0.42
1:C:469:LEU:HD21	1:D:468:LEU:HD11	2.02	0.42
1:H:559:PRO:HD3	1:H:572:VAL:HG12	2.01	0.41
1:E:525:ARG:HB3	1:E:539:GLU:OE2	2.20	0.41
1:H:579:ARG:NH1	1:H:603:GLU:OE1	2.51	0.41
1:G:497:LEU:HD12	1:G:591:VAL:HG12	2.03	0.41
1:B:551:SER:HB3	1:F:476:MET:CE	2.51	0.41
1:F:476:MET:HE3	1:F:482:THR:HA	2.02	0.41
1:C:557:LEU:HB2	1:C:578:LEU:HD11	2.03	0.41
1:G:506:CYS:HB2	1:G:509:TYR:CZ	2.56	0.41
1:G:472:MET:C	1:G:474:VAL:N	2.75	0.41
1:G:469:LEU:HA	1:G:469:LEU:HD12	1.93	0.41
1:B:472:MET:CB	1:B:474:VAL:HG23	2.46	0.40
1:F:538:GLU:HG3	1:F:539:GLU:N	2.36	0.40
1:B:475:ALA:HB2	1:B:486:PHE:CE2	2.56	0.40
1:F:537:LYS:HD3	1:F:563:ALA:HA	2.03	0.40
1:E:482:THR:HG21	1:F:472:MET:HE1	2.03	0.40
1:E:518:VAL:HG11	1:E:586:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ARG:NH1	1:B:520:ARG:CG	2.64	0.40
1:G:472:MET:SD	1:G:472:MET:N	2.95	0.40
1:C:478:GLU:HG3	1:C:478:GLU:H	1.61	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	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
1	B	138/154 (90%)	134 (97%)	4 (3%)	0	100	100
1	C	149/154 (97%)	142 (95%)	7 (5%)	0	100	100
1	D	146/154 (95%)	142 (97%)	4 (3%)	0	100	100
1	E	146/154 (95%)	143 (98%)	3 (2%)	0	100	100
1	F	149/154 (97%)	141 (95%)	7 (5%)	1 (1%)	26	14
1	G	144/154 (94%)	133 (92%)	8 (6%)	3 (2%)	9	1
1	H	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	26	14
All	All	1176/1232 (96%)	1129 (96%)	42 (4%)	5 (0%)	39	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	523	GLY
1	G	550	GLY
1	H	524	GLU
1	G	548	ARG
1	F	533	GLY

### 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	132/132 (100%)	129 (98%)	3 (2%)	58	51
1	B	122/132 (92%)	109 (89%)	13 (11%)	8	3
1	C	129/132 (98%)	120 (93%)	9 (7%)	19	8
1	D	127/132 (96%)	122 (96%)	5 (4%)	39	27
1	E	127/132 (96%)	124 (98%)	3 (2%)	57	49
1	F	129/132 (98%)	120 (93%)	9 (7%)	19	8
1	G	125/132 (95%)	113 (90%)	12 (10%)	10	3
1	H	132/132 (100%)	130 (98%)	2 (2%)	72	69
All	All	1023/1056 (97%)	967 (94%)	56 (6%)	27	14

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	LEU
1	A	526	ARG
1	A	548	ARG
1	B	465	ARG
1	B	466	GLU
1	B	471	GLU
1	B	476	MET
1	B	482	THR
1	B	515	ILE
1	B	520	ARG
1	B	527	GLN
1	B	538	GLU
1	B	558	GLU
1	B	570	LYS
1	B	602	GLN
1	B	603	GLU
1	C	478	GLU
1	C	508	LEU
1	C	512	LYS

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Mol	Chain	Res	Type
1	C	521	GLU
1	C	524	GLU
1	C	526	ARG
1	C	576	SER
1	C	603	GLU
1	C	604	ARG
1	D	459	GLU
1	D	461	ILE
1	D	478	GLU
1	D	579	ARG
1	D	580	SER
1	E	522	ASP
1	E	544	ARG
1	E	580	SER
1	F	476	MET
1	F	508	LEU
1	F	522	ASP
1	F	524	GLU
1	F	534	HIS
1	F	561	GLU
1	F	571	LYS
1	F	576	SER
1	F	596	HIS
1	G	463	MET
1	G	468	LEU
1	G	469	LEU
1	G	479	ASP
1	G	490	LYS
1	G	525	ARG
1	G	526	ARG
1	G	530	VAL
1	G	547	SER
1	G	551	SER
1	G	570	LYS
1	G	601	ARG
1	H	504	SER
1	H	548	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	527	GLN

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Mol	Chain	Res	Type
1	B	582	ASN
1	B	595	ASN
1	B	602	GLN
1	C	590	HIS
1	G	527	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	154/154 (100%)	0.12	5 (3%) 51 54	17, 29, 67, 121	0
1	B	142/154 (92%)	0.47	13 (9%) 11 12	23, 45, 89, 108	0
1	C	151/154 (98%)	0.26	10 (6%) 22 24	19, 36, 87, 147	0
1	D	148/154 (96%)	0.18	8 (5%) 29 33	19, 36, 115, 250	0
1	E	148/154 (96%)	0.12	8 (5%) 29 33	19, 35, 87, 137	0
1	F	151/154 (98%)	0.29	13 (8%) 13 14	21, 36, 95, 149	0
1	G	146/154 (94%)	0.65	21 (14%) 3 4	24, 46, 112, 163	0
1	H	154/154 (100%)	0.12	6 (3%) 43 47	17, 28, 74, 135	0
All	All	1194/1232 (96%)	0.27	84 (7%) 19 21	17, 37, 94, 250	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	480	GLY	9.0
1	C	478	GLU	7.6
1	E	522	ASP	7.0
1	F	522	ASP	6.6
1	G	524	GLU	5.9
1	A	549	GLY	5.8
1	G	522	ASP	5.5
1	D	521	GLU	5.2
1	D	522	ASP	5.2
1	H	549	GLY	5.1
1	G	479	ASP	5.1
1	G	523	GLY	5.0
1	G	525	ARG	5.0
1	A	548	ARG	5.0
1	D	524	GLU	4.8
1	E	524	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	550	GLY	4.7
1	F	480	GLY	4.7
1	F	478	GLU	4.5
1	F	479	ASP	4.3
1	C	480	GLY	4.3
1	H	548	ARG	4.2
1	G	526	ARG	4.2
1	G	470	ALA	4.1
1	C	550	GLY	4.1
1	B	561	GLU	4.1
1	B	472	MET	3.9
1	G	548	ARG	3.8
1	F	550	GLY	3.6
1	G	561	GLU	3.4
1	G	549	GLY	3.2
1	B	478	GLU	3.2
1	G	480	GLY	3.1
1	A	522	ASP	3.1
1	F	603	GLU	3.1
1	E	525	ARG	3.1
1	B	549	GLY	3.0
1	F	524	GLU	3.0
1	H	524	GLU	2.9
1	E	521	GLU	2.9
1	F	526	ARG	2.9
1	A	607	THR	2.9
1	B	520	ARG	2.9
1	H	607	THR	2.8
1	E	547	SER	2.8
1	D	548	ARG	2.8
1	G	551	SER	2.8
1	C	522	ASP	2.7
1	E	551	SER	2.7
1	E	523	GLY	2.7
1	G	550	GLY	2.7
1	E	546	ASP	2.6
1	C	549	GLY	2.6
1	H	523	GLY	2.6
1	C	604	ARG	2.6
1	G	473	GLY	2.6
1	B	548	ARG	2.6
1	C	534	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	523	GLY	2.6
1	D	526	ARG	2.6
1	B	480	GLY	2.5
1	G	467	ALA	2.5
1	F	604	ARG	2.5
1	G	562	GLY	2.5
1	B	551	SER	2.5
1	H	522	ASP	2.4
1	G	468	LEU	2.4
1	F	547	SER	2.4
1	B	473	GLY	2.3
1	D	525	ARG	2.3
1	F	534	HIS	2.3
1	F	549	GLY	2.3
1	G	478	GLU	2.3
1	C	523	GLY	2.3
1	G	601	ARG	2.3
1	C	561	GLU	2.2
1	G	521	GLU	2.1
1	B	476	MET	2.1
1	B	538	GLU	2.1
1	F	525	ARG	2.1
1	B	474	VAL	2.0
1	B	562	GLY	2.0
1	C	603	GLU	2.0
1	G	533	GLY	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.