



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:16 pm BST

PDB ID : 6G52  
Title : CRYSTAL STRUCTURE OF THE CNMP BINDING DOMAIN OF THE MAGNESIUM TRANSPORTER CNNM4  
Authors : Gimenez, P.; Oyenarte, I.; Hardy, S.; Zubillaga, M.; Merino, N.; Blanco, F.J.; Siliqi, D.; Tremblay, M.; Muller, D.; Martinez-Cruz, L.A.  
Deposited on : 2018-03-28  
Resolution : 3.69 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

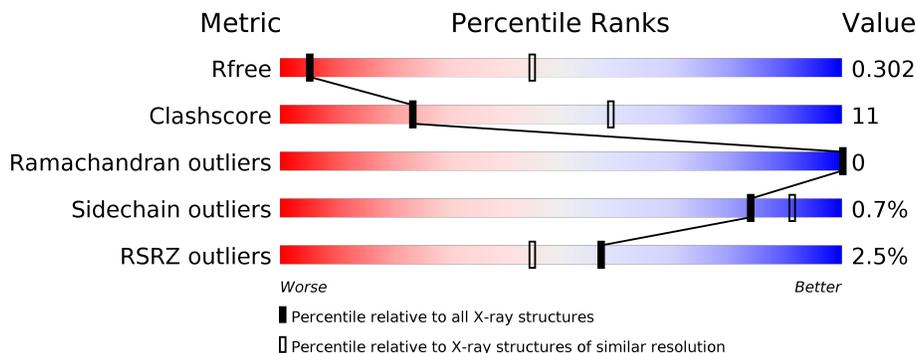
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.69 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))
$R_{free}$	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 respectively. 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	189	
1	B	189	
1	C	189	
1	D	189	
1	E	189	
1	F	189	

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Mol	Chain	Length	Quality of chain
1	G	189	<p>%</p> <p>54% 20% 26%</p>
1	H	189	<p>55% 19% 26%</p>
1	I	189	<p>7%</p> <p>65% 7% 28%</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9252 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 Metal transporter CNNM4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	I	137	Total 870	C 558	N 145	O 164	Se 3	0	0	0
1	B	150	Total 1132	C 732	N 189	O 207	Se 4	0	0	0
1	C	136	Total 1016	C 660	N 167	O 186	Se 3	0	0	0
1	D	136	Total 986	C 642	N 157	O 184	Se 3	0	0	0
1	E	138	Total 1036	C 672	N 168	O 192	Se 4	0	0	0
1	F	136	Total 1054	C 685	N 175	O 191	Se 3	0	0	0
1	G	139	Total 1051	C 677	N 179	O 191	Se 4	0	0	0
1	H	139	Total 1039	C 678	N 168	O 189	Se 4	0	0	0
1	A	138	Total 1068	C 692	N 175	O 197	Se 4	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

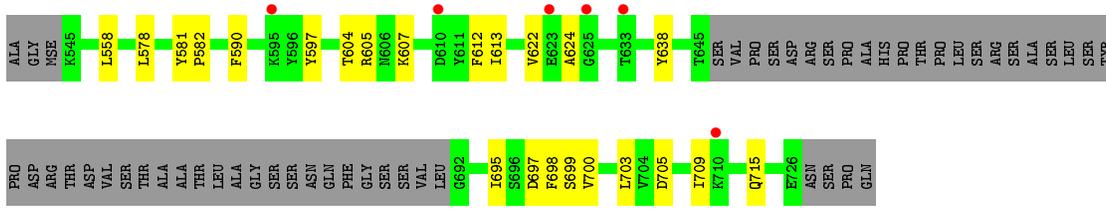
Chain	Residue	Modelled	Actual	Comment	Reference
I	542	ALA	-	expression tag	UNP Q6P4Q7
I	543	GLY	-	expression tag	UNP Q6P4Q7
I	544	MSE	-	expression tag	UNP Q6P4Q7
B	542	ALA	-	expression tag	UNP Q6P4Q7
B	543	GLY	-	expression tag	UNP Q6P4Q7
B	544	MSE	-	expression tag	UNP Q6P4Q7
C	542	ALA	-	expression tag	UNP Q6P4Q7
C	543	GLY	-	expression tag	UNP Q6P4Q7
C	544	MSE	-	expression tag	UNP Q6P4Q7
D	542	ALA	-	expression tag	UNP Q6P4Q7
D	543	GLY	-	expression tag	UNP Q6P4Q7

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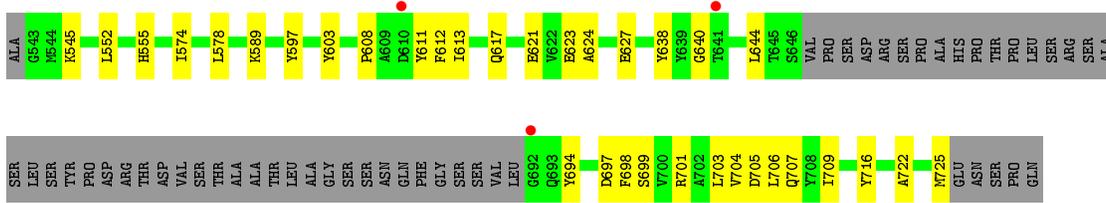
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Chain	Residue	Modelled	Actual	Comment	Reference
D	544	MSE	-	expression tag	UNP Q6P4Q7
E	542	ALA	-	expression tag	UNP Q6P4Q7
E	543	GLY	-	expression tag	UNP Q6P4Q7
E	544	MSE	-	expression tag	UNP Q6P4Q7
F	542	ALA	-	expression tag	UNP Q6P4Q7
F	543	GLY	-	expression tag	UNP Q6P4Q7
F	544	MSE	-	expression tag	UNP Q6P4Q7
G	542	ALA	-	expression tag	UNP Q6P4Q7
G	543	GLY	-	expression tag	UNP Q6P4Q7
G	544	MSE	-	expression tag	UNP Q6P4Q7
H	542	ALA	-	expression tag	UNP Q6P4Q7
H	543	GLY	-	expression tag	UNP Q6P4Q7
H	544	MSE	-	expression tag	UNP Q6P4Q7
A	542	ALA	-	expression tag	UNP Q6P4Q7
A	543	GLY	-	expression tag	UNP Q6P4Q7
A	544	MSE	-	expression tag	UNP Q6P4Q7

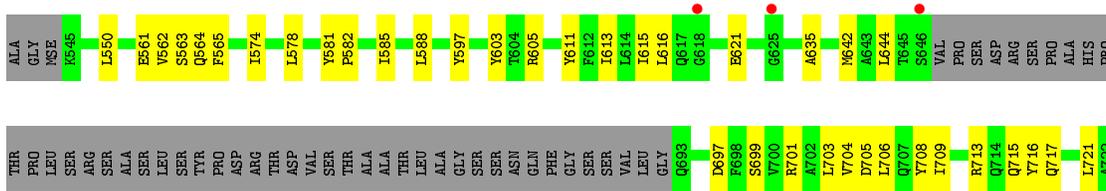




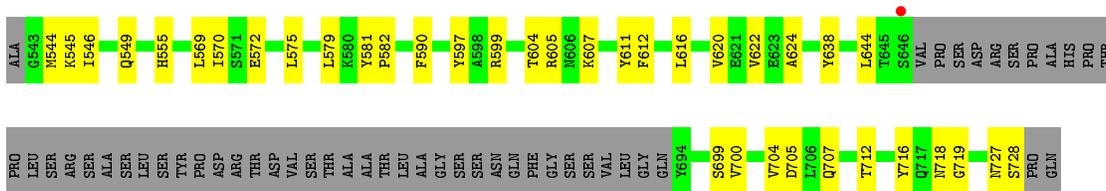
• Molecule 1: Metal transporter CNNM4



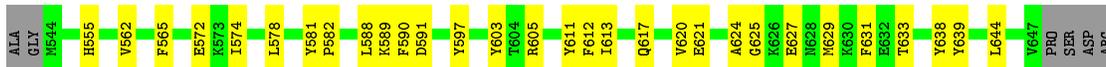
• Molecule 1: Metal transporter CNNM4



• Molecule 1: Metal transporter CNNM4



• Molecule 1: Metal transporter CNNM4





- Molecule 1: Metal transporter CNNM4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.74Å 116.74Å 243.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.29 – 3.69 93.37 – 3.69	Depositor EDS
% Data completeness (in resolution range)	96.8 (63.29-3.69) 96.9 (93.37-3.69)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.67Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.284 , 0.303 0.284 , 0.302	Depositor DCC
$R_{free}$ test set	1991 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	9252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.28	0/1087	0.52	0/1466
1	B	0.25	0/1151	0.44	0/1554
1	C	0.25	0/1034	0.54	0/1401
1	D	0.26	0/1004	0.46	0/1363
1	E	0.25	0/1054	0.48	0/1423
1	F	0.27	0/1074	0.54	0/1453
1	G	0.26	0/1069	0.51	0/1444
1	H	0.27	0/1059	0.48	0/1435
1	I	0.26	0/881	0.48	0/1202
All	All	0.26	0/9413	0.50	0/12741

There are no bond length outliers.

There are no bond angle outliers.

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	1068	0	1008	29	0
1	B	1132	0	1050	19	0
1	C	1016	0	935	33	0
1	D	986	0	864	14	0
1	E	1036	0	955	24	0
1	F	1054	0	993	27	0
1	G	1051	0	969	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1039	0	947	23	0
1	I	870	0	664	10	0
All	All	9252	0	8385	198	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 11.

All (198) 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:F:616:LEU:HD11	1:F:709:ILE:HG23	1.56	0.86
1:C:612:PHE:HE1	1:C:638:TYR:HB2	1.41	0.86
1:C:616:LEU:HD11	1:C:709:ILE:HG23	1.58	0.85
1:C:624:ALA:HB2	1:C:698:PHE:HA	1.62	0.81
1:A:555:HIS:HE1	1:A:572:GLU:HG3	1.47	0.79
1:F:562:VAL:HG11	1:F:565:PHE:HD2	1.52	0.75
1:G:546:ILE:HD12	1:G:616:LEU:HD13	1.71	0.72
1:G:605:ARG:HG2	1:G:699:SER:HB2	1.70	0.71
1:A:569:LEU:HD13	1:A:720:LEU:HD23	1.71	0.70
1:F:605:ARG:HG3	1:F:699:SER:HB2	1.72	0.70
1:A:555:HIS:CE1	1:A:572:GLU:HG3	2.27	0.69
1:B:704:VAL:O	1:B:706:LEU:HD23	1.91	0.69
1:B:605:ARG:HG3	1:B:699:SER:HB2	1.75	0.68
1:B:558:LEU:HD11	1:B:614:LEU:HD13	1.75	0.67
1:B:633:THR:HG22	1:B:634:GLY:H	1.60	0.67
1:B:704:VAL:HG12	1:B:705:ASP:H	1.59	0.67
1:F:550:LEU:HD11	1:F:616:LEU:HB3	1.77	0.67
1:E:617:GLN:HG2	1:E:707:GLN:HB2	1.77	0.66
1:A:569:LEU:HD13	1:A:720:LEU:CD2	2.26	0.66
1:B:620:VAL:HG23	1:B:702:ALA:HA	1.78	0.64
1:I:555:HIS:CE1	1:I:572:GLU:HG3	2.32	0.64
1:F:621:GLU:OE1	1:F:701:ARG:NH2	2.31	0.63
1:A:564:GLN:O	1:A:569:LEU:HD12	1.98	0.63
1:G:612:PHE:HE1	1:G:638:TYR:HB2	1.63	0.63
1:H:603:TYR:HE1	1:H:613:ILE:HG12	1.64	0.62
1:E:574:ILE:O	1:E:578:LEU:HB2	2.00	0.61
1:H:617:GLN:HG2	1:H:707:GLN:HB2	1.83	0.61
1:F:713:ARG:O	1:F:717:GLN:HG2	2.00	0.61
1:D:605:ARG:HG3	1:D:699:SER:HB3	1.83	0.61
1:H:629:MSE:HG3	1:H:631:PHE:CZ	2.37	0.60
1:A:704:VAL:HG12	1:A:705:ASP:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:581:TYR:CD1	1:G:582:PRO:HD2	2.36	0.60
1:C:556:ARG:HG3	1:A:556:ARG:HB3	1.83	0.59
1:G:644:LEU:HB3	1:G:716:TYR:CD2	2.37	0.59
1:D:612:PHE:HE2	1:D:638:TYR:HB2	1.67	0.59
1:F:588:LEU:HD23	1:F:706:LEU:HD21	1.83	0.59
1:G:612:PHE:CE1	1:G:638:TYR:HB2	2.38	0.58
1:A:555:HIS:CD2	1:A:575:LEU:HB3	2.39	0.58
1:H:621:GLU:HA	1:H:631:PHE:O	2.04	0.57
1:F:615:ILE:HG22	1:F:635:ALA:HA	1.87	0.57
1:G:704:VAL:HG12	1:G:705:ASP:H	1.70	0.57
1:D:612:PHE:CE2	1:D:638:TYR:HB2	2.40	0.57
1:C:558:LEU:HD21	1:C:565:PHE:CD2	2.40	0.56
1:H:612:PHE:HE1	1:H:638:TYR:HB2	1.70	0.56
1:H:621:GLU:HB2	1:H:703:LEU:HD21	1.87	0.56
1:B:627:GLU:HG2	1:A:642:MSE:HG3	1.88	0.56
1:C:578:LEU:HD21	1:C:711:ILE:HG23	1.87	0.56
1:I:615:ILE:O	1:I:636:PHE:N	2.32	0.56
1:E:612:PHE:CE1	1:E:638:TYR:HB2	2.41	0.55
1:C:566:SER:HB2	1:C:569:LEU:HD23	1.87	0.55
1:H:620:VAL:HG22	1:H:633:THR:HG22	1.87	0.55
1:C:712:THR:HB	1:C:715:GLN:HG3	1.89	0.55
1:C:555:HIS:CE1	1:C:572:GLU:HG3	2.42	0.55
1:C:615:ILE:O	1:C:636:PHE:N	2.26	0.54
1:G:611:TYR:HB3	1:G:712:THR:HG22	1.89	0.54
1:A:622:VAL:O	1:A:630:LYS:HA	2.07	0.54
1:B:624:ALA:HB2	1:B:698:PHE:HB3	1.89	0.54
1:A:571:SER:H	1:A:723:SER:HB2	1.72	0.54
1:E:621:GLU:OE1	1:E:701:ARG:NH2	2.40	0.54
1:F:644:LEU:O	1:F:717:GLN:NE2	2.38	0.54
1:E:704:VAL:HG12	1:E:705:ASP:N	2.23	0.54
1:G:575:LEU:HD13	1:G:579:LEU:HD13	1.90	0.54
1:C:704:VAL:HG12	1:C:705:ASP:N	2.24	0.53
1:A:704:VAL:HG12	1:A:705:ASP:N	2.24	0.53
1:F:697:ASP:OD1	1:F:697:ASP:N	2.41	0.53
1:E:612:PHE:HE1	1:E:638:TYR:HB2	1.74	0.52
1:F:616:LEU:HD12	1:F:708:TYR:HA	1.90	0.52
1:E:623:GLU:HB3	1:E:699:SER:HB3	1.91	0.51
1:F:644:LEU:HB3	1:F:716:TYR:CD2	2.45	0.51
1:D:695:ILE:HD12	1:G:727:ASN:H	1.75	0.51
1:H:627:GLU:HB2	1:H:629:MSE:HE2	1.92	0.51
1:F:721:LEU:HA	1:F:724:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:605:ARG:HH21	1:G:624:ALA:HA	1.75	0.51
1:G:590:PHE:N	1:G:705:ASP:OD1	2.31	0.51
1:C:605:ARG:HG2	1:C:699:SER:HB2	1.92	0.50
1:E:574:ILE:O	1:E:578:LEU:CB	2.59	0.50
1:B:704:VAL:HG12	1:B:705:ASP:N	2.24	0.50
1:F:581:TYR:CD1	1:F:582:PRO:HD2	2.46	0.50
1:G:555:HIS:ND1	1:G:575:LEU:HD12	2.26	0.50
1:G:604:THR:HG23	1:G:607:LYS:CB	2.42	0.50
1:H:605:ARG:HH12	1:H:624:ALA:HA	1.75	0.50
1:C:704:VAL:HG12	1:C:705:ASP:H	1.76	0.50
1:F:613:ILE:HA	1:F:709:ILE:O	2.12	0.49
1:A:644:LEU:HB3	1:A:716:TYR:CD2	2.46	0.49
1:D:613:ILE:HA	1:D:709:ILE:O	2.12	0.49
1:E:722:ALA:HA	1:E:725:MSE:HE3	1.94	0.49
1:B:544:MSE:HA	1:G:545:LYS:HE2	1.95	0.49
1:H:612:PHE:HB3	1:H:644:LEU:HD21	1.94	0.49
1:G:544:MSE:HE2	1:G:707:GLN:HG3	1.94	0.49
1:A:562:VAL:HG11	1:A:565:PHE:HD2	1.78	0.49
1:D:624:ALA:HB2	1:D:698:PHE:HB3	1.94	0.49
1:D:578:LEU:HD21	1:D:715:GLN:HB3	1.95	0.49
1:H:625:GLY:HA3	1:H:629:MSE:HE3	1.93	0.49
1:C:574:ILE:HD12	1:C:723:SER:HA	1.95	0.48
1:H:633:THR:HG21	1:H:639:TYR:OH	2.13	0.48
1:A:605:ARG:HG3	1:A:699:SER:HB2	1.95	0.48
1:F:562:VAL:HG11	1:F:565:PHE:CD2	2.39	0.48
1:G:620:VAL:HG21	1:G:700:VAL:HG13	1.96	0.48
1:E:608:PRO:HA	1:E:694:TYR:O	2.14	0.48
1:E:603:TYR:OH	1:E:611:TYR:O	2.31	0.47
1:G:622:VAL:HA	1:G:699:SER:O	2.13	0.47
1:H:562:VAL:HG23	1:H:565:PHE:HB2	1.96	0.47
1:H:612:PHE:CE1	1:H:638:TYR:HB2	2.48	0.47
1:I:608:PRO:HA	1:I:695:ILE:HA	1.95	0.47
1:G:569:LEU:HD13	1:G:570:ILE:HG13	1.96	0.47
1:G:704:VAL:HG12	1:G:705:ASP:N	2.28	0.47
1:D:697:ASP:N	1:D:697:ASP:OD1	2.48	0.47
1:F:581:TYR:CG	1:F:582:PRO:HD2	2.50	0.47
1:F:603:TYR:OH	1:F:611:TYR:O	2.30	0.47
1:D:581:TYR:CG	1:D:582:PRO:HD2	2.49	0.47
1:D:604:THR:HG23	1:D:607:LYS:CB	2.45	0.47
1:C:716:TYR:CZ	1:C:720:LEU:HD11	2.50	0.47
1:D:703:LEU:HD23	1:D:703:LEU:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:627:GLU:HG2	1:F:642:MSE:SE	2.65	0.46
1:C:553:ALA:HB2	1:A:557:PHE:CD1	2.51	0.46
1:C:603:TYR:OH	1:C:611:TYR:O	2.28	0.46
1:C:716:TYR:O	1:C:720:LEU:HG	2.16	0.46
1:F:578:LEU:HD11	1:F:715:GLN:HB3	1.98	0.46
1:C:558:LEU:O	1:C:562:VAL:HB	2.16	0.46
1:B:589:LYS:CB	1:G:582:PRO:HB3	2.46	0.46
1:B:621:GLU:OE2	1:B:630:LYS:HB3	2.16	0.46
1:F:704:VAL:HG12	1:F:705:ASP:N	2.31	0.46
1:A:581:TYR:HD2	1:A:584:VAL:HG23	1.81	0.46
1:G:597:TYR:CD2	1:G:599:ARG:HG2	2.50	0.46
1:G:644:LEU:HD22	1:G:716:TYR:HB2	1.98	0.45
1:B:581:TYR:CG	1:B:582:PRO:HD2	2.51	0.45
1:F:562:VAL:HG12	1:F:565:PHE:H	1.81	0.45
1:B:642:MSE:HG2	1:A:627:GLU:HG3	1.98	0.45
1:H:588:LEU:HB3	1:H:706:LEU:HD12	1.98	0.45
1:E:624:ALA:HB2	1:E:698:PHE:HA	1.99	0.45
1:A:619:LYS:O	1:A:703:LEU:HB2	2.17	0.45
1:E:704:VAL:HG12	1:E:705:ASP:H	1.81	0.45
1:E:621:GLU:HB3	1:E:703:LEU:HD11	1.99	0.45
1:G:549:GLN:OE1	1:G:549:GLN:N	2.43	0.45
1:I:578:LEU:O	1:I:584:VAL:HG21	2.17	0.45
1:D:622:VAL:HG12	1:D:700:VAL:HG22	1.99	0.45
1:F:563:SER:HB2	1:F:564:GLN:NE2	2.32	0.45
1:D:590:PHE:N	1:D:705:ASP:OD1	2.27	0.44
1:A:697:ASP:OD1	1:A:698:PHE:N	2.51	0.44
1:A:571:SER:OG	1:A:574:ILE:HG12	2.18	0.44
1:F:574:ILE:HD12	1:F:723:SER:HA	1.98	0.44
1:G:611:TYR:HA	1:G:712:THR:HA	1.99	0.44
1:B:567:PRO:HA	1:B:570:ILE:O	2.18	0.44
1:C:556:ARG:CG	1:A:556:ARG:HB3	2.46	0.44
1:C:613:ILE:O	1:C:613:ILE:HG13	2.18	0.44
1:C:614:LEU:HD23	1:C:638:TYR:HB3	1.98	0.44
1:E:545:LYS:HB3	1:E:545:LYS:HE2	1.82	0.44
1:C:604:THR:O	1:C:696:SER:OG	2.35	0.44
1:H:574:ILE:O	1:H:578:LEU:HB2	2.18	0.44
1:C:701:ARG:NH1	1:C:703:LEU:HD23	2.32	0.43
1:G:597:TYR:HD2	1:G:599:ARG:HG2	1.83	0.43
1:G:546:ILE:CD1	1:G:616:LEU:HD13	2.45	0.43
1:H:555:HIS:NE2	1:H:572:GLU:HG3	2.33	0.43
1:C:712:THR:HG22	1:C:714:GLN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:718:ASN:OD1	1:G:719:GLY:N	2.52	0.43
1:A:575:LEU:O	1:A:579:LEU:HD13	2.18	0.43
1:C:709:ILE:HG13	1:C:709:ILE:O	2.18	0.43
1:F:585:ILE:HG13	1:F:709:ILE:HG22	2.00	0.43
1:I:574:ILE:O	1:I:578:LEU:HB2	2.19	0.43
1:C:636:PHE:CD2	1:A:550:LEU:HD12	2.54	0.43
1:C:621:GLU:HB3	1:C:703:LEU:HD11	2.01	0.43
1:A:544:MSE:HE1	1:A:705:ASP:HB3	2.01	0.43
1:E:589:LYS:HE3	1:E:589:LYS:HB3	1.86	0.42
1:E:617:GLN:O	1:E:706:LEU:HD23	2.19	0.42
1:H:605:ARG:NH1	1:H:697:ASP:O	2.52	0.42
1:D:558:LEU:HD11	1:D:709:ILE:HD11	2.02	0.42
1:A:581:TYR:CG	1:A:582:PRO:HD2	2.53	0.42
1:F:561:GLU:O	1:F:562:VAL:HG23	2.19	0.42
1:C:642:MSE:HG3	1:C:694:TYR:HE2	1.83	0.42
1:H:603:TYR:OH	1:H:611:TYR:O	2.29	0.42
1:C:644:LEU:HB3	1:C:716:TYR:CD2	2.53	0.42
1:E:697:ASP:N	1:E:697:ASP:OD1	2.50	0.42
1:I:584:VAL:O	1:I:710:LYS:N	2.33	0.42
1:A:602:LEU:O	1:A:611:TYR:OH	2.27	0.42
1:B:569:LEU:HD12	1:B:569:LEU:HA	1.89	0.42
1:E:613:ILE:HA	1:E:709:ILE:O	2.20	0.42
1:G:727:ASN:HB3	1:G:728:SER:H	1.75	0.42
1:A:613:ILE:HA	1:A:709:ILE:O	2.19	0.42
1:B:589:LYS:HE3	1:B:589:LYS:HB3	1.80	0.42
1:H:589:LYS:HB3	1:H:589:LYS:HE3	1.86	0.42
1:B:589:LYS:NZ	1:B:705:ASP:OD2	2.46	0.41
1:B:574:ILE:O	1:B:578:LEU:HB2	2.19	0.41
1:H:581:TYR:CG	1:H:582:PRO:HD2	2.55	0.41
1:I:567:PRO:HA	1:I:570:ILE:O	2.20	0.41
1:E:552:LEU:HA	1:E:555:HIS:ND1	2.36	0.41
1:G:555:HIS:NE2	1:G:572:GLU:HG3	2.35	0.41
1:I:697:ASP:OD1	1:I:697:ASP:N	2.50	0.41
1:I:555:HIS:NE2	1:I:572:GLU:HG3	2.35	0.41
1:F:621:GLU:HB2	1:F:703:LEU:CD1	2.49	0.41
1:C:613:ILE:HA	1:C:709:ILE:O	2.20	0.41
1:E:612:PHE:HB3	1:E:644:LEU:HD21	2.02	0.41
1:E:603:TYR:OH	1:E:640:GLY:HA3	2.21	0.41
1:E:644:LEU:HB3	1:E:716:TYR:CD2	2.56	0.40
1:A:564:GLN:OE1	1:A:641:THR:OG1	2.38	0.40
1:C:612:PHE:HB2	1:C:640:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:LYS:O	1:C:711:ILE:HD13	2.21	0.40
1:H:590:PHE:HB2	1:H:705:ASP:N	2.36	0.40
1:I:582:PRO:HG3	1:H:591:ASP:HA	2.04	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	134/189 (71%)	134 (100%)	0	0	100	100
1	B	146/189 (77%)	142 (97%)	4 (3%)	0	100	100
1	C	132/189 (70%)	130 (98%)	2 (2%)	0	100	100
1	D	132/189 (70%)	132 (100%)	0	0	100	100
1	E	134/189 (71%)	134 (100%)	0	0	100	100
1	F	132/189 (70%)	132 (100%)	0	0	100	100
1	G	135/189 (71%)	130 (96%)	5 (4%)	0	100	100
1	H	135/189 (71%)	135 (100%)	0	0	100	100
1	I	133/189 (70%)	132 (99%)	1 (1%)	0	100	100
All	All	1213/1701 (71%)	1201 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	105/160 (66%)	104 (99%)	1 (1%)	76	86
1	B	106/160 (66%)	105 (99%)	1 (1%)	78	88
1	C	94/160 (59%)	94 (100%)	0	100	100
1	D	85/160 (53%)	84 (99%)	1 (1%)	71	84
1	E	97/160 (61%)	96 (99%)	1 (1%)	76	86
1	F	102/160 (64%)	101 (99%)	1 (1%)	76	86
1	G	98/160 (61%)	98 (100%)	0	100	100
1	H	95/160 (59%)	94 (99%)	1 (1%)	73	85
1	I	55/160 (34%)	55 (100%)	0	100	100
All	All	837/1440 (58%)	831 (99%)	6 (1%)	84	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	597	TYR
1	D	597	TYR
1	E	597	TYR
1	F	597	TYR
1	H	597	TYR
1	A	597	TYR

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

### 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	134/189 (70%)	0.14	1 (0%) 87 81	54, 89, 118, 143	0
1	B	146/189 (77%)	0.23	2 (1%) 75 64	47, 82, 130, 157	0
1	C	133/189 (70%)	0.44	1 (0%) 86 78	69, 112, 147, 159	0
1	D	133/189 (70%)	0.53	6 (4%) 33 24	75, 109, 139, 151	0
1	E	134/189 (70%)	0.31	3 (2%) 62 50	61, 95, 123, 169	0
1	F	133/189 (70%)	0.39	3 (2%) 60 48	67, 100, 129, 155	0
1	G	135/189 (71%)	0.26	1 (0%) 87 81	57, 93, 118, 138	0
1	H	135/189 (71%)	0.29	0 100 100	64, 92, 129, 151	0
1	I	133/189 (70%)	0.78	13 (9%) 7 6	96, 133, 172, 189	0
All	All	1216/1701 (71%)	0.37	30 (2%) 57 45	47, 100, 143, 189	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	598	ALA	4.6
1	I	591	ASP	4.5
1	C	582	PRO	4.1
1	A	646	SER	3.6
1	D	633	THR	3.5
1	E	610	ASP	3.0
1	F	646	SER	2.9
1	I	593	HIS	2.9
1	B	693	GLN	2.8
1	I	631	PHE	2.8
1	I	560	THR	2.7
1	I	624	ALA	2.6
1	E	641	THR	2.6
1	D	710	LYS	2.5
1	I	545	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	623	GLU	2.2
1	I	634	GLY	2.2
1	F	625	GLY	2.2
1	I	610	ASP	2.2
1	D	610	ASP	2.2
1	I	563	SER	2.2
1	D	625	GLY	2.2
1	B	563	SER	2.2
1	E	692	GLY	2.2
1	I	698	PHE	2.2
1	I	575	LEU	2.1
1	F	618	GLY	2.1
1	I	594	ASN	2.1
1	D	595	LYS	2.0
1	G	646	SER	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.