



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:04 AM UTC

PDB ID : 6G52 / pdb_00006g52
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

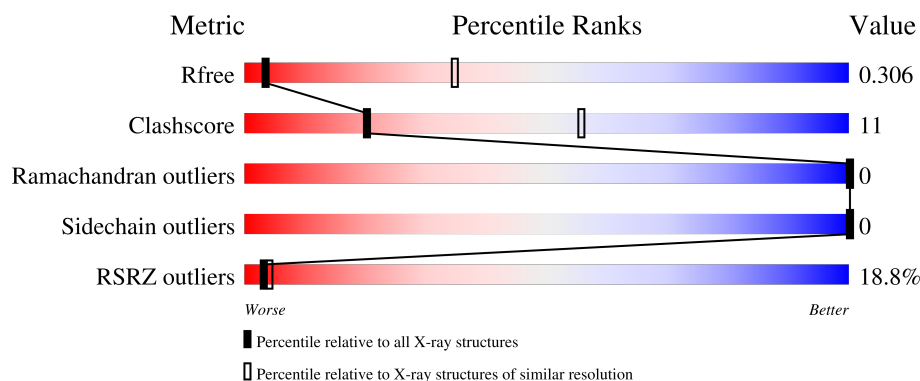
1 Overall quality at a glance

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.



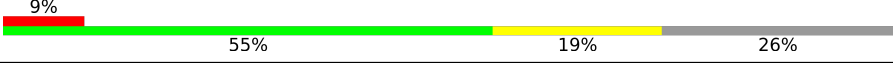
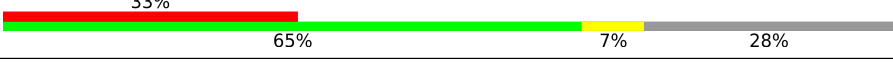
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	7% 53% 20% 27%
1	B	189	11% 66% 14% 21%
1	C	189	16% 49% 23% 28%
1	D	189	10% 60% 12% 28%
1	E	189	11% 56% 17% 27%

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Mol	Chain	Length	Quality of chain
1	F	189	
1	G	189	
1	H	189	
1	I	189	

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

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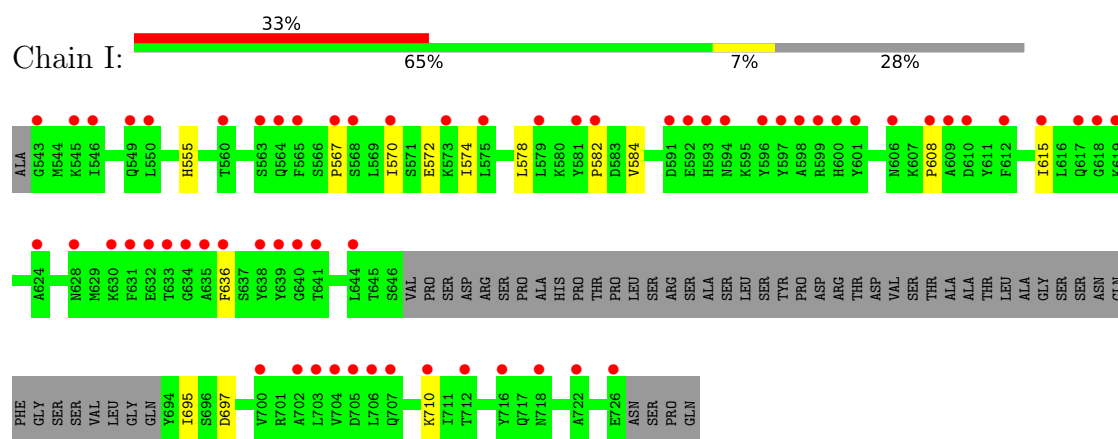
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Chain	Residue	Modelled	Actual	Comment	Reference
D	544	MSE	-	expression tag	UNP Q6P4Q7
E	542	ALA	-	expression tag	UNP Q6P4Q7
E	543	GLY	-	expression tag	UNP Q6P4Q7
E	544	MSE	-	expression tag	UNP Q6P4Q7
F	542	ALA	-	expression tag	UNP Q6P4Q7
F	543	GLY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

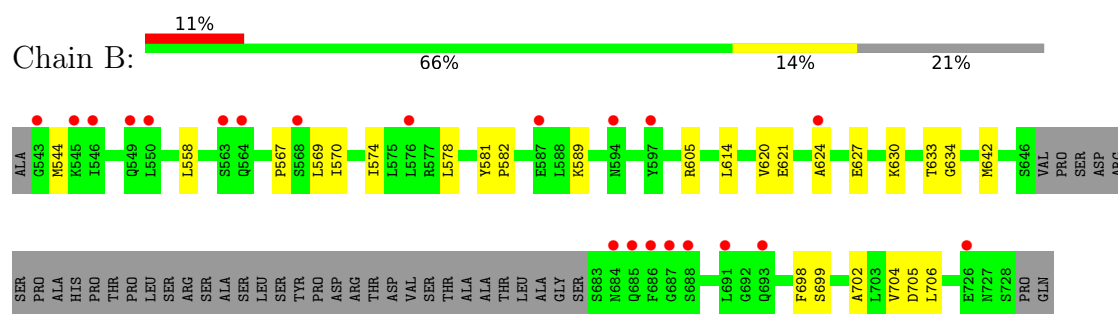
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

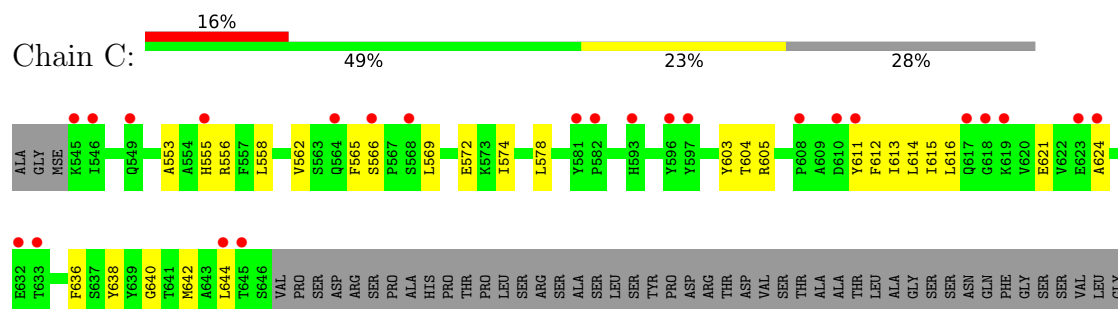
• Molecule 1: Metal transporter CNNM4



• Molecule 1: Metal transporter CNNM4

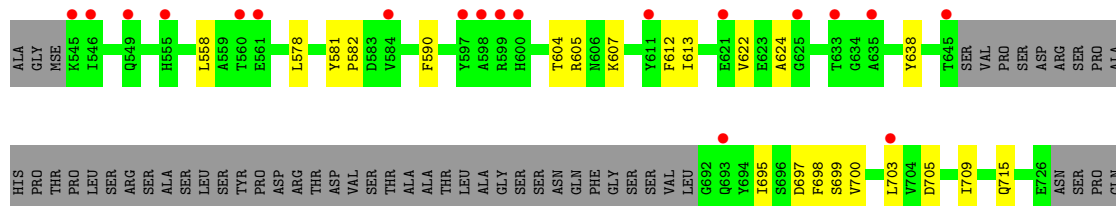


• Molecule 1: Metal transporter CNNM4

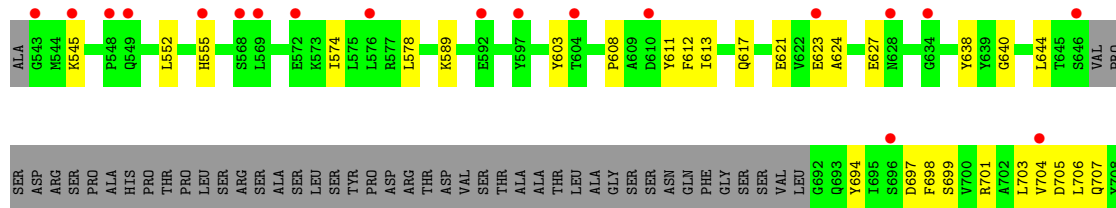




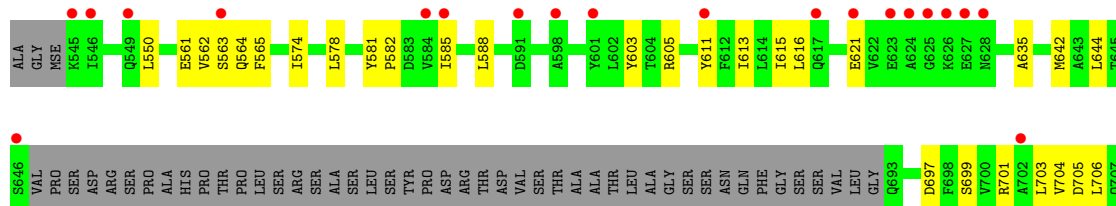
- Molecule 1: Metal transporter CNNM4



- Molecule 1: Metal transporter CNNM4

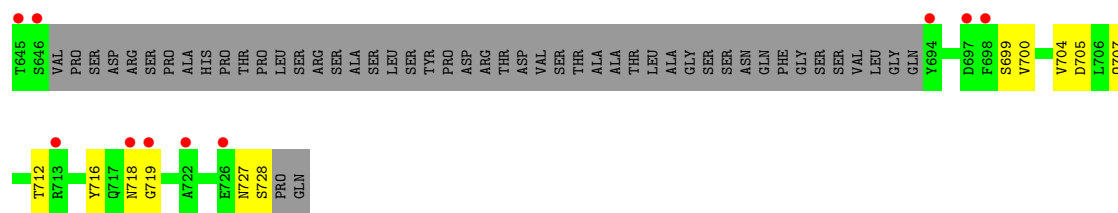


- Molecule 1: Metal transporter CNNM4

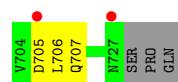
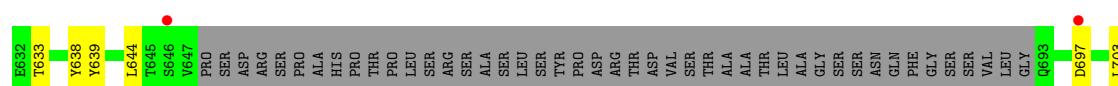
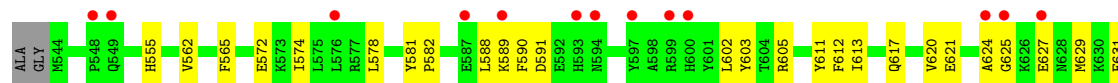


- Molecule 1: Metal transporter CNNM4

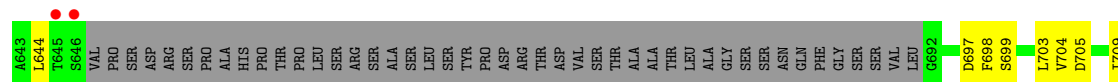
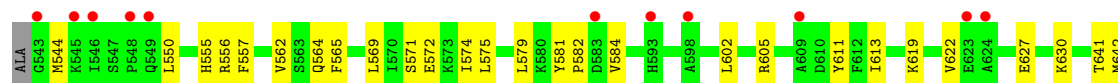




● Molecule 1: Metal transporter CNNM4



● 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, α , β , γ	116.74Å 116.74Å 243.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.29 – 3.69 63.29 – 3.69	Depositor EDS
% Data completeness (in resolution range)	96.8 (63.29-3.69) 96.9 (63.29-3.69)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.284 , 0.303 0.285 , 0.306	Depositor DCC
R_{free} test set	1991 reflections (9.32%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	9252	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.22	0/1087	0.46	0/1466
1	B	0.12	0/1151	0.37	0/1554
1	C	0.18	0/1034	0.47	0/1401
1	D	0.12	0/1004	0.36	0/1363
1	E	0.14	0/1054	0.41	0/1423
1	F	0.18	0/1074	0.49	0/1453
1	G	0.17	0/1069	0.47	0/1444
1	H	0.15	0/1059	0.42	0/1435
1	I	0.14	0/881	0.46	0/1202
All	All	0.16	0/9413	0.44	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	24	0
1	I	870	0	664	10	0
All	All	9252	0	8385	199	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 (199) 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:F:605:ARG:HG3	1:F:699:SER:HB2	1.72	0.70
1:A:569:LEU:HD13	1:A:720:LEU:HD23	1.71	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:I:615:ILE:O	1:I:636:PHE:N	2.32	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: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:B:624:ALA:HB2	1:B:698:PHE:HB3	1.89	0.54
1:A:622:VAL:O	1:A:630:LYS:HA	2.07	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:590:PHE:N	1:G:705:ASP:OD1	2.31	0.51
1:G:605:ARG:HH21	1:G:624:ALA:HA	1.75	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:D:613:ILE:HA	1:D:709:ILE:O	2.12	0.49
1:A:644:LEU:HB3	1:A:716:TYR:CD2	2.46	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:B:589:LYS:NZ	1:B:705:ASP:OD2	2.46	0.49
1:D:578:LEU:HD21	1:D:715:GLN:HB3	1.95	0.49
1:D:624:ALA:HB2	1:D:698:PHE:HB3	1.94	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:H:602:LEU:O	1:H:611:TYR:OH	2.28	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:I:608:PRO:HA	1:I:695:ILE:HA	1.95	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:704:VAL:HG12	1:E:705:ASP:H	1.81	0.45
1:A:619:LYS:O	1:A:703:LEU:HB2	2.17	0.45
1:I:578:LEU:O	1:I:584:VAL:HG21	2.17	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: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: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:A:571:SER:OG	1:A:574:ILE:HG12	2.18	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:HE2	1:E:545:LYS:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:574:ILE:O	1:I:578:LEU:HB2	2.19	0.43
1:C:709:ILE:O	1:C:709:ILE:HG13	2.18	0.43
1:F:585:ILE:HG13	1:F:709:ILE:HG22	2.00	0.43
1:C:621:GLU:HB3	1:C:703:LEU:HD11	2.01	0.43
1:C:636:PHE:CD2	1:A:550:LEU:HD12	2.54	0.43
1:A:544:MSE:HE1	1:A:705:ASP:HB3	2.01	0.43
1:E:589:LYS:HB3	1:E:589:LYS:HE3	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:F:561:GLU:O	1:F:562:VAL:HG23	2.19	0.42
1:A:581:TYR:CG	1:A:582:PRO:HD2	2.53	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:I:584:VAL:O	1:I:710:LYS:N	2.33	0.42
1:C:644:LEU:HB3	1:C:716:TYR:CD2	2.53	0.42
1:E:697:ASP:OD1	1:E:697:ASP:N	2.50	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:602:LEU:O	1:A:611:TYR:OH	2.27	0.42
1:B:589:LYS:HB3	1:B:589:LYS:HE3	1.80	0.42
1:H:589:LYS:HB3	1:H:589:LYS:HE3	1.86	0.42
1:A:613:ILE:HA	1:A:709:ILE:O	2.19	0.42
1:I:567:PRO:HA	1:I:570:ILE:O	2.20	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:697:ASP:OD1	1:I:697:ASP:N	2.50	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: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:603:TYR:OH	1:E:640:GLY:HA3	2.21	0.41
1:E:612:PHE:HB3	1:E:644:LEU:HD21	2.02	0.41
1:E:644:LEU:HB3	1:E:716:TYR:CD2	2.56	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:A:564:GLN:OE1	1:A:641:THR:OG1	2.38	0.40
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%)	105 (100%)	0	100	100
1	B	106/160 (66%)	106 (100%)	0	100	100
1	C	94/160 (59%)	94 (100%)	0	100	100
1	D	85/160 (53%)	85 (100%)	0	100	100
1	E	97/160 (61%)	97 (100%)	0	100	100
1	F	102/160 (64%)	102 (100%)	0	100	100
1	G	98/160 (61%)	98 (100%)	0	100	100
1	H	95/160 (59%)	95 (100%)	0	100	100
1	I	55/160 (34%)	55 (100%)	0	100	100
All	All	837/1440 (58%)	837 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	B	564	GLN
1	D	564	GLN
1	F	617	GLN
1	F	715	GLN
1	H	617	GLN
1	H	707	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	134/189 (70%)	1.15	13 (9%) 13 13	54, 89, 118, 143	0
1	B	146/189 (77%)	1.11	21 (14%) 6 8	47, 82, 130, 157	0
1	C	133/189 (70%)	1.48	30 (22%) 2 3	69, 112, 147, 159	0
1	D	133/189 (70%)	1.37	19 (14%) 6 8	75, 109, 139, 151	0
1	E	134/189 (70%)	1.20	20 (14%) 5 7	61, 95, 123, 169	0
1	F	133/189 (70%)	1.36	22 (16%) 4 6	67, 100, 129, 155	0
1	G	135/189 (71%)	1.28	24 (17%) 4 5	57, 93, 118, 138	0
1	H	135/189 (71%)	1.27	17 (12%) 8 9	64, 92, 129, 151	0
1	I	133/189 (70%)	2.17	63 (47%) 0 1	96, 133, 172, 189	0
All	All	1216/1701 (71%)	1.37	229 (18%) 3 4	47, 100, 143, 189	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	543	GLY	5.3
1	I	600	HIS	4.8
1	I	565	PHE	4.7
1	I	598	ALA	4.6
1	D	549	GLN	4.2
1	I	705	ASP	4.2
1	I	702	ALA	4.2
1	D	600	HIS	4.1
1	I	704	VAL	4.1
1	I	630	LYS	3.9
1	C	623	GLU	3.9
1	C	611	TYR	3.9
1	I	599	ARG	3.8
1	I	631	PHE	3.8
1	B	563	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	633	THR	3.7
1	E	568	SER	3.7
1	I	549	GLN	3.7
1	I	632	GLU	3.7
1	I	716	TYR	3.6
1	I	617	GLN	3.6
1	G	543	GLY	3.6
1	I	634	GLY	3.6
1	F	591	ASP	3.5
1	E	549	GLN	3.4
1	D	693	GLN	3.4
1	I	644	LEU	3.4
1	C	597	TYR	3.4
1	I	641	THR	3.4
1	I	610	ASP	3.4
1	B	685	GLN	3.4
1	A	623	GLU	3.3
1	C	715	GLN	3.3
1	I	601	TYR	3.3
1	A	543	GLY	3.3
1	H	627	GLU	3.3
1	B	693	GLN	3.3
1	F	584	VAL	3.3
1	B	546	ILE	3.2
1	C	582	PRO	3.2
1	F	545	LYS	3.2
1	I	597	TYR	3.2
1	F	624	ALA	3.2
1	A	548	PRO	3.2
1	I	564	GLN	3.1
1	I	707	GLN	3.1
1	I	608	PRO	3.1
1	H	589	LYS	3.1
1	G	585	ILE	3.0
1	G	713	ARG	3.0
1	I	550	LEU	3.0
1	H	697	ASP	3.0
1	I	700	VAL	3.0
1	G	726	GLU	3.0
1	H	597	TYR	3.0
1	G	623	GLU	3.0
1	I	612	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	543	GLY	3.0
1	I	560	THR	2.9
1	C	546	ILE	2.9
1	F	628	ASN	2.9
1	A	646	SER	2.9
1	F	598	ALA	2.9
1	G	604	THR	2.9
1	A	545	LYS	2.9
1	I	635	ALA	2.8
1	E	555	HIS	2.8
1	I	710	LYS	2.8
1	E	610	ASP	2.8
1	C	726	GLU	2.8
1	B	726	GLU	2.7
1	I	606	ASN	2.7
1	I	579	LEU	2.7
1	B	686	PHE	2.7
1	I	618	GLY	2.7
1	I	640	GLY	2.7
1	C	564	GLN	2.7
1	C	617	GLN	2.7
1	D	598	ALA	2.7
1	D	560	THR	2.7
1	I	546	ILE	2.7
1	B	587	GLU	2.7
1	F	646	SER	2.7
1	G	698	PHE	2.7
1	C	632	GLU	2.7
1	E	604	THR	2.7
1	H	727	ASN	2.7
1	I	593	HIS	2.7
1	G	610	ASP	2.7
1	D	546	ILE	2.7
1	F	601	TYR	2.7
1	G	633	THR	2.7
1	I	706	LEU	2.7
1	H	646	SER	2.7
1	A	546	ILE	2.6
1	A	549	GLN	2.6
1	I	722	ALA	2.6
1	A	624	ALA	2.6
1	D	621	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	621	GLU	2.6
1	E	592	GLU	2.6
1	H	599	ARG	2.6
1	D	635	ALA	2.6
1	F	549	GLN	2.6
1	I	543	GLY	2.6
1	C	618	GLY	2.6
1	I	624	ALA	2.6
1	C	593	HIS	2.5
1	C	596	TYR	2.5
1	I	592	GLU	2.5
1	E	576	LEU	2.5
1	I	594	ASN	2.5
1	B	594	ASN	2.5
1	G	591	ASP	2.5
1	E	548	PRO	2.5
1	H	549	GLN	2.5
1	I	545	LYS	2.5
1	E	545	LYS	2.5
1	I	568	SER	2.5
1	C	568	SER	2.5
1	F	627	GLU	2.5
1	C	624	ALA	2.5
1	D	545	LYS	2.5
1	D	645	THR	2.5
1	G	718	ASN	2.4
1	I	567	PRO	2.4
1	I	712	THR	2.4
1	G	646	SER	2.4
1	G	694	TYR	2.4
1	A	645	THR	2.4
1	I	596	TYR	2.4
1	I	638	TYR	2.4
1	G	548	PRO	2.4
1	B	687	GLY	2.4
1	I	591	ASP	2.4
1	I	581	TYR	2.4
1	F	623	GLU	2.4
1	G	640	GLY	2.4
1	F	611	TYR	2.4
1	I	609	ALA	2.4
1	A	593	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	628	ASN	2.3
1	F	710	LYS	2.3
1	I	575	LEU	2.3
1	G	719	GLY	2.3
1	D	599	ARG	2.3
1	I	639	TYR	2.3
1	I	703	LEU	2.3
1	D	703	LEU	2.3
1	H	576	LEU	2.3
1	F	625	GLY	2.3
1	H	593	HIS	2.3
1	G	545	LYS	2.3
1	A	609	ALA	2.3
1	G	697	ASP	2.3
1	I	636	PHE	2.3
1	E	623	GLU	2.3
1	F	726	GLU	2.3
1	C	566	SER	2.3
1	B	549	GLN	2.3
1	D	611	TYR	2.3
1	B	568	SER	2.3
1	C	619	LYS	2.3
1	B	684	ASN	2.2
1	G	645	THR	2.2
1	C	608	PRO	2.2
1	D	625	GLY	2.2
1	I	563	SER	2.2
1	E	597	TYR	2.2
1	I	726	GLU	2.2
1	I	582	PRO	2.2
1	C	644	LEU	2.2
1	H	548	PRO	2.2
1	I	619	LYS	2.2
1	I	718	ASN	2.2
1	B	545	LYS	2.2
1	F	702	ALA	2.2
1	G	722	ALA	2.2
1	B	688	SER	2.2
1	E	634	GLY	2.2
1	G	619	LYS	2.2
1	D	555	HIS	2.2
1	E	572	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	727	ASN	2.2
1	H	705	ASP	2.1
1	I	615	ILE	2.1
1	D	561	GLU	2.1
1	C	633	THR	2.1
1	C	645	THR	2.1
1	G	641	THR	2.1
1	B	550	LEU	2.1
1	B	564	GLN	2.1
1	C	549	GLN	2.1
1	C	714	GLN	2.1
1	E	696	SER	2.1
1	E	723	SER	2.1
1	C	610	ASP	2.1
1	A	583	ASP	2.1
1	B	624	ALA	2.1
1	H	624	ALA	2.1
1	F	617	GLN	2.1
1	D	584	VAL	2.1
1	F	626	LYS	2.1
1	H	600	HIS	2.1
1	B	597	TYR	2.1
1	C	708	TYR	2.1
1	B	576	LEU	2.1
1	G	627	GLU	2.1
1	I	570	ILE	2.1
1	F	546	ILE	2.1
1	F	585	ILE	2.1
1	C	545	LYS	2.1
1	I	573	LYS	2.1
1	E	646	SER	2.1
1	F	563	SER	2.1
1	A	598	ALA	2.1
1	D	633	THR	2.0
1	H	587	GLU	2.0
1	C	703	LEU	2.0
1	E	569	LEU	2.0
1	E	628	ASN	2.0
1	H	625	GLY	2.0
1	C	581	TYR	2.0
1	D	597	TYR	2.0
1	B	691	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	594	ASN	2.0
1	G	599	ARG	2.0
1	C	555	HIS	2.0
1	E	704	VAL	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 oligosaccharides 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.