



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:08 AM GMT

PDB ID : 1D0N  
Title : THE CRYSTAL STRUCTURE OF CALCIUM-FREE EQUINE PLASMA GELSOLIN.  
Authors : Burtnick, L.D.; Robinson, R.; Li, C.  
Deposited on : 1999-09-13  
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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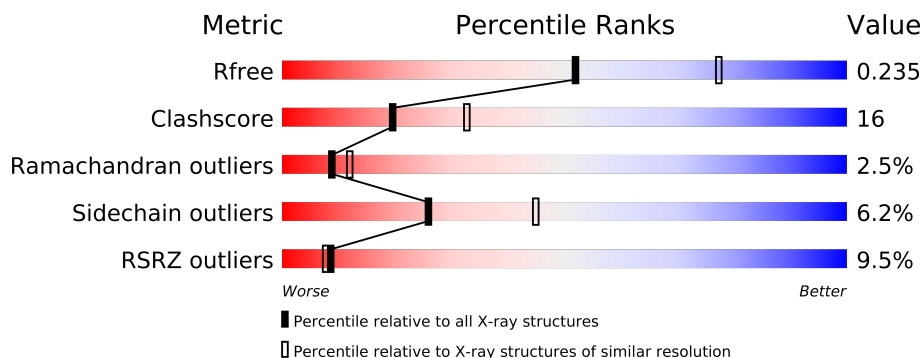
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	729	
1	B	729	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11666 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HORSE PLASMA GELSOLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5691	3598	990	1087	16			
1	B	729	Total	C	N	O	S	0	0	0
			5691	3598	990	1087	16			

- Molecule 2 is water.

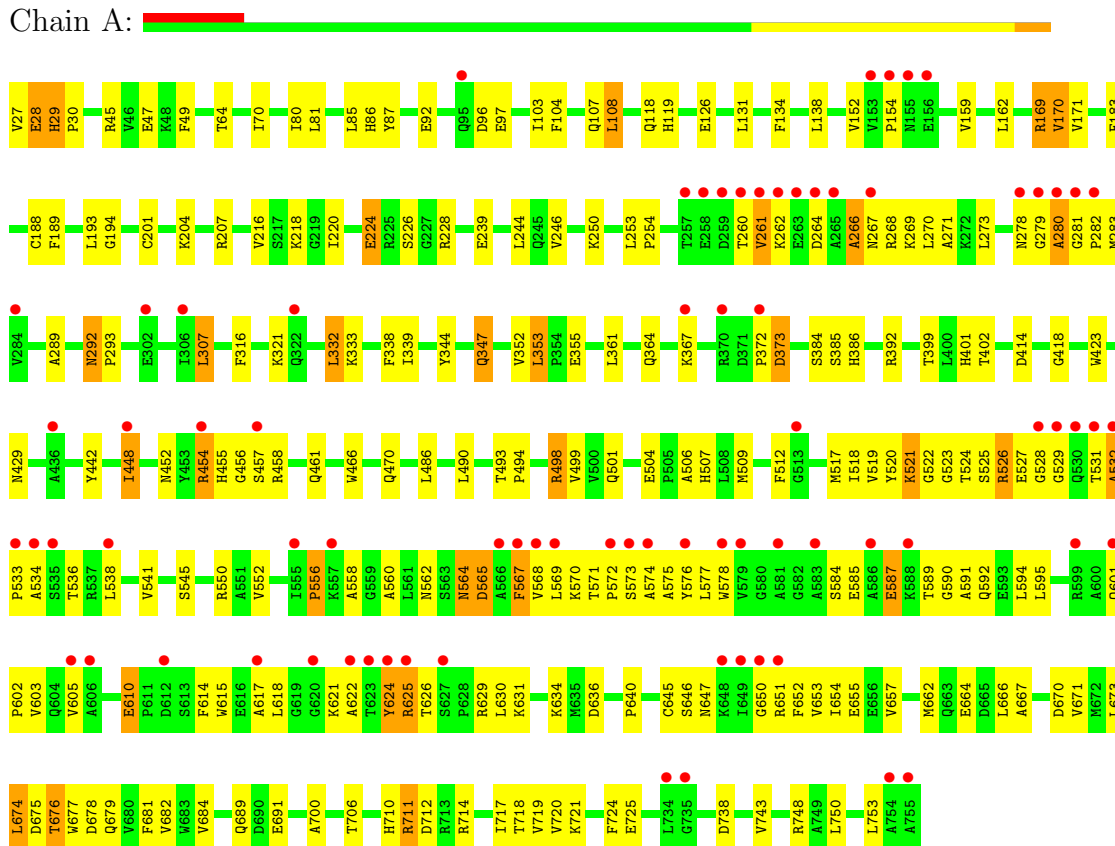
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		
2	B	145	Total	O	0	0
			145	145		

### 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.

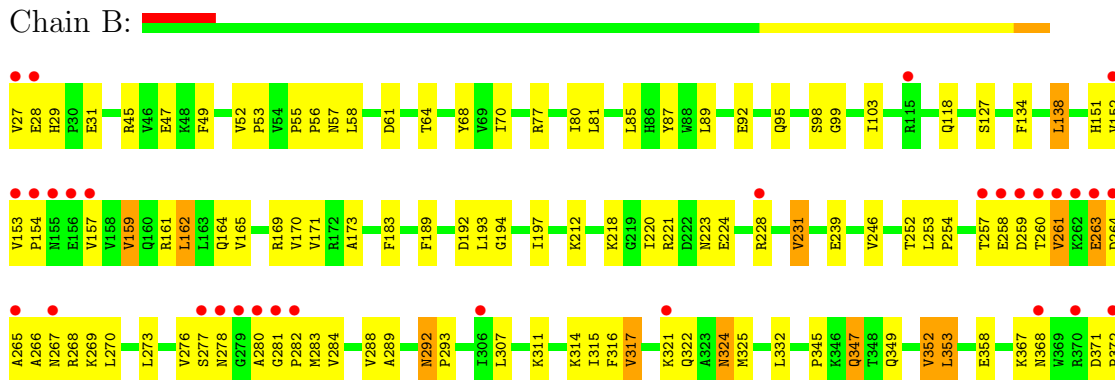
#### • Molecule 1: HORSE PLASMA GELSOLIN

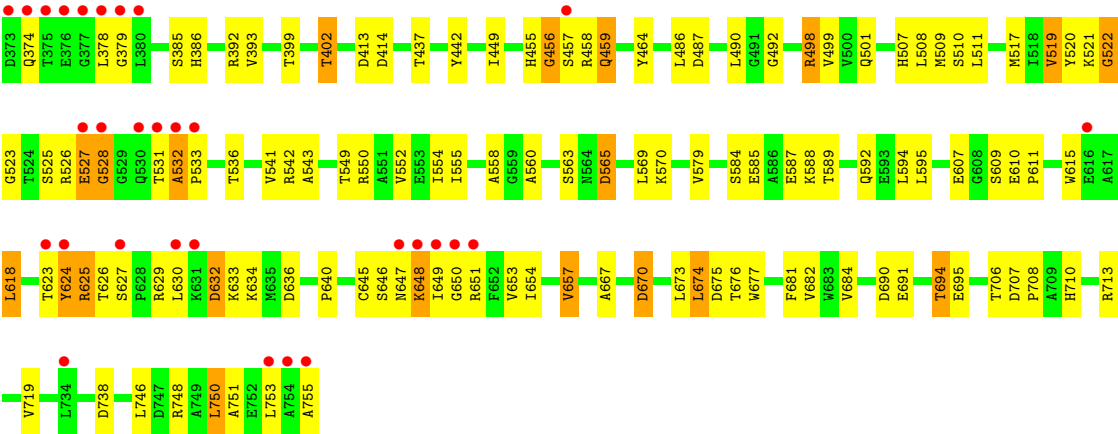
Chain A:



#### • Molecule 1: HORSE PLASMA GELSOLIN

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.40Å 169.40Å 154.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.50) 91.9 (19.98-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.50Å)	Xtriage
Refinement program	X-PLOR, CNS	Depositor
R, $R_{free}$	0.205 , 0.238 0.204 , 0.235	Depositor DCC
$R_{free}$ test set	3617 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	0 of 71389 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11666	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 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.35	0/5825	0.59	2/7894 (0.0%)
1	B	0.37	0/5825	0.61	0/7894
All	All	0.36	0/11650	0.60	2/15788 (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	A	676	THR	N-CA-C	-5.48	96.21	111.00
1	A	224	GLU	N-CA-C	-5.14	97.12	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5691	0	5547	185	0
1	B	5691	0	5547	178	0
2	A	139	0	0	7	0
2	B	145	0	0	4	0
All	All	11666	0	11094	363	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (363) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:118:GLN:HB2	1:B:352:VAL:HG13	1.50	0.93
1:B:579:VAL:HG21	1:B:588:LYS:HE2	1.53	0.90
1:B:29:HIS:HD2	1:B:31:GLU:H	1.20	0.89
1:A:399:THR:O	1:A:402:THR:HG22	1.77	0.83
1:A:118:GLN:HB2	1:A:352:VAL:HG22	1.59	0.83
1:A:592:GLN:HA	1:A:595:LEU:HD23	1.63	0.81
1:B:558:ALA:HA	1:B:618:LEU:HD23	1.64	0.80
1:B:353:LEU:HD12	1:B:358:GLU:HA	1.64	0.79
1:A:578:TRP:HA	1:A:605:VAL:HG13	1.68	0.76
1:A:278:ASN:HB3	1:A:283:MET:HA	1.67	0.76
1:B:153:VAL:HG12	1:B:157:VAL:HG21	1.69	0.75
1:B:508:LEU:HG	1:B:517:MET:CE	2.18	0.74
1:A:169:ARG:HG3	1:A:655:GLU:OE2	1.88	0.73
1:A:307:LEU:HB3	1:A:316:PHE:HB2	1.71	0.73
1:B:293:PRO:HD3	1:B:710:HIS:ND1	2.03	0.73
1:B:261:VAL:HG13	1:B:263:GLU:HG2	1.70	0.73
1:A:442:TYR:HB3	1:A:523:GLY:O	1.88	0.72
1:B:267:ASN:O	1:B:268:ARG:HD3	1.91	0.71
1:A:571:THR:HG23	1:A:573:SER:H	1.54	0.71
1:B:675:ASP:OD1	1:B:676:THR:O	2.10	0.70
1:B:508:LEU:HG	1:B:517:MET:HE1	1.73	0.70
1:B:353:LEU:HD23	1:B:353:LEU:N	2.08	0.69
1:A:97:GLU:HG3	2:A:796:HOH:O	1.92	0.68
1:B:64:THR:CG2	1:B:92:GLU:HG2	2.25	0.67
1:A:269:LYS:HB3	1:A:706:THR:O	1.93	0.67
1:A:571:THR:HG22	1:A:574:ALA:O	1.94	0.67
1:A:501:GLN:HE21	1:A:519:VAL:CG1	2.08	0.67
1:B:292:ASN:HD22	1:B:292:ASN:H	1.43	0.67
1:A:647:ASN:ND2	1:A:652:PHE:HD1	1.93	0.67
1:A:455:HIS:O	1:A:457:SER:N	2.28	0.66
1:A:339:ILE:HG23	1:A:344:TYR:HB2	1.77	0.66
1:A:292:ASN:HD22	1:A:292:ASN:H	1.42	0.66
1:B:170:VAL:HA	2:B:799:HOH:O	1.94	0.66
1:A:675:ASP:OD1	1:A:676:THR:O	2.13	0.66
1:B:623:THR:HG22	1:B:624:TYR:H	1.61	0.66
1:A:571:THR:OG1	1:A:572:PRO:HD2	1.95	0.66
1:A:239:GLU:CD	1:A:239:GLU:H	1.99	0.66
1:A:646:SER:HB2	1:A:653:VAL:HG12	1.78	0.65
1:B:317:VAL:HG22	1:B:352:VAL:HB	1.79	0.65
1:A:629:ARG:HH11	1:A:629:ARG:HG3	1.62	0.64
1:A:293:PRO:HD3	1:A:710:HIS:ND1	2.12	0.64
1:A:266:ALA:HB2	1:A:651:ARG:HH11	1.63	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:585:GLU:O	1:A:589:THR:HG22	1.97	0.63
1:B:151:HIS:O	1:B:153:VAL:HG23	1.98	0.63
1:A:682:VAL:HG13	1:A:719:VAL:HA	1.80	0.63
1:A:712:ASP:OD2	1:A:714:ARG:HB2	1.99	0.63
1:B:265:ALA:HA	1:B:268:ARG:HE	1.64	0.62
1:B:263:GLU:O	1:B:265:ALA:N	2.31	0.62
1:B:584:SER:H	1:B:587:GLU:HG2	1.65	0.62
1:A:526:ARG:HG3	1:A:527:GLU:HG2	1.82	0.62
1:B:269:LYS:HB3	1:B:706:THR:O	2.00	0.62
1:B:345:PRO:HB3	1:B:347:GLN:OE1	2.00	0.61
1:A:126:GLU:HG2	1:A:131:LEU:HD21	1.82	0.61
1:B:347:GLN:CD	1:B:347:GLN:H	2.02	0.61
1:A:504:GLU:HG2	1:A:517:MET:CE	2.30	0.61
1:B:676:THR:HG22	1:B:677:TRP:H	1.66	0.61
1:B:630:LEU:O	1:B:634:LYS:HB2	2.01	0.61
1:B:713:ARG:HB3	1:B:713:ARG:NH2	2.16	0.61
1:A:676:THR:HG22	1:A:677:TRP:N	2.16	0.60
1:B:648:LYS:HG2	1:B:649:ILE:HG12	1.83	0.60
1:B:584:SER:H	1:B:587:GLU:CG	2.14	0.60
1:B:623:THR:HG22	1:B:624:TYR:N	2.16	0.60
1:B:588:LYS:O	1:B:592:GLN:HG2	2.02	0.60
1:A:647:ASN:HD21	1:A:652:PHE:HD1	1.48	0.59
1:B:542:ARG:HE	1:B:629:ARG:NH2	2.01	0.59
1:B:29:HIS:CD2	1:B:31:GLU:H	2.12	0.59
1:A:442:TYR:CD2	1:A:525:SER:HB3	2.38	0.59
1:B:266:ALA:HB2	1:B:651:ARG:HG3	1.85	0.59
1:B:278:ASN:HB3	1:B:283:MET:HA	1.84	0.59
1:A:626:THR:HG22	1:A:626:THR:O	2.02	0.59
1:A:575:ALA:HB3	1:A:602:PRO:HA	1.84	0.59
1:B:273:LEU:O	1:B:288:VAL:HG22	2.03	0.59
1:B:321:LYS:HG3	1:B:322:GLN:HG3	1.85	0.59
1:A:267:ASN:O	1:A:268:ARG:HD3	2.03	0.59
1:B:239:GLU:H	1:B:239:GLU:CD	2.07	0.58
1:B:748:ARG:O	1:B:751:ALA:HB3	2.04	0.58
1:B:292:ASN:ND2	1:B:292:ASN:H	2.01	0.58
1:B:153:VAL:CG1	1:B:157:VAL:HG21	2.34	0.58
1:A:260:THR:HG22	1:A:261:VAL:HG23	1.85	0.58
1:B:414:ASP:OD2	1:B:507:HIS:HE1	1.87	0.57
1:A:170:VAL:HA	2:A:849:HOH:O	2.04	0.57
1:A:278:ASN:CB	1:A:283:MET:HA	2.35	0.57
1:A:562:ASN:HB3	1:A:565:ASP:OD1	2.05	0.57
1:A:700:ALA:HB3	1:A:717:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:ARG:HD3	1:A:47:GLU:OE2	2.05	0.56
1:A:64:THR:CG2	1:A:92:GLU:HG2	2.36	0.56
1:A:550:ARG:NH1	1:A:552:VAL:HG21	2.21	0.56
1:A:753:LEU:H	1:A:753:LEU:HD22	1.71	0.56
1:A:414:ASP:OD2	1:A:507:HIS:HE1	1.89	0.56
1:A:423:TRP:HB2	1:A:448:ILE:HG23	1.88	0.56
1:B:542:ARG:HE	1:B:629:ARG:CZ	2.18	0.56
1:A:401:HIS:HB3	2:A:768:HOH:O	2.05	0.56
1:B:442:TYR:CD2	1:B:525:SER:HB3	2.41	0.56
1:A:605:VAL:HG21	1:A:610:GLU:HB3	1.88	0.55
1:A:509:MET:SD	1:A:550:ARG:HD3	2.46	0.55
1:B:442:TYR:HB3	1:B:523:GLY:O	2.05	0.55
1:B:292:ASN:HA	1:B:293:PRO:C	2.27	0.55
1:A:662:MET:HB3	1:A:664:GLU:OE1	2.06	0.55
1:A:228:ARG:NH1	1:A:228:ARG:HB3	2.21	0.55
1:B:676:THR:HG22	1:B:677:TRP:N	2.20	0.55
1:A:541:VAL:O	1:A:565:ASP:HB2	2.06	0.55
1:B:691:GLU:O	1:B:694:THR:HG22	2.06	0.55
1:A:753:LEU:HD22	1:A:753:LEU:N	2.22	0.55
1:A:466:TRP:HA	1:A:499:VAL:HG13	1.89	0.55
1:A:347:GLN:CD	1:A:347:GLN:H	2.09	0.55
1:B:64:THR:HG22	1:B:92:GLU:HG2	1.89	0.54
1:A:521:LYS:HB2	1:A:521:LYS:NZ	2.23	0.54
1:B:682:VAL:HG13	1:B:719:VAL:HA	1.88	0.54
1:A:584:SER:H	1:A:587:GLU:CG	2.21	0.54
1:A:682:VAL:HG11	1:A:719:VAL:HG22	1.89	0.54
1:A:682:VAL:CG1	1:A:719:VAL:HG22	2.38	0.54
1:A:293:PRO:HD3	1:A:710:HIS:CE1	2.43	0.53
1:A:448:ILE:HD11	1:A:486:LEU:HD23	1.90	0.53
1:A:279:GLY:O	1:A:280:ALA:HB2	2.08	0.53
1:A:152:VAL:HG22	1:A:154:PRO:HD3	1.90	0.53
1:B:508:LEU:HG	1:B:517:MET:HE3	1.90	0.53
1:B:27:VAL:O	1:B:28:GLU:HB2	2.07	0.53
1:B:455:HIS:O	1:B:457:SER:N	2.41	0.53
1:B:647:ASN:HA	1:B:651:ARG:O	2.08	0.53
1:A:458:ARG:HG3	1:A:458:ARG:HH11	1.73	0.53
1:A:646:SER:HB2	1:A:653:VAL:CG1	2.39	0.53
1:B:706:THR:O	1:B:706:THR:HG22	2.10	0.52
1:B:276:VAL:HG13	1:B:276:VAL:O	2.09	0.52
1:B:385:SER:HB2	2:B:774:HOH:O	2.09	0.52
1:B:519:VAL:HG13	1:B:552:VAL:HA	1.90	0.52
1:A:504:GLU:HG2	1:A:517:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:527:GLU:HG3	1:A:528:GLY:N	2.25	0.52
1:A:27:VAL:C	1:A:28:GLU:HG2	2.30	0.52
1:B:70:ILE:N	1:B:70:ILE:HD12	2.26	0.51
1:B:80:ILE:HG22	1:B:81:LEU:N	2.25	0.51
1:A:568:VAL:HG22	1:A:577:LEU:HD12	1.92	0.51
1:A:601:GLN:NE2	1:A:601:GLN:HA	2.24	0.51
1:A:498:ARG:NH1	1:A:498:ARG:O	2.44	0.51
1:A:418:GLY:HA2	1:A:454:ARG:NH2	2.26	0.51
1:B:281:GLY:H	1:B:282:PRO:CD	2.24	0.51
1:A:292:ASN:H	1:A:292:ASN:ND2	2.09	0.51
1:A:518:ILE:HD12	1:A:594:LEU:HD13	1.93	0.51
1:A:654:ILE:O	1:A:654:ILE:HG13	2.10	0.51
1:A:527:GLU:HG3	1:A:528:GLY:H	1.75	0.50
1:B:442:TYR:CE2	1:B:525:SER:HB3	2.46	0.50
1:B:392:ARG:NH2	1:B:636:ASP:OD1	2.44	0.50
1:A:281:GLY:H	1:A:282:PRO:HD2	1.76	0.50
1:A:571:THR:HG23	1:A:573:SER:N	2.25	0.50
1:B:684:VAL:HG23	1:B:684:VAL:O	2.11	0.50
1:B:293:PRO:HG2	1:B:367:LYS:HE2	1.93	0.50
1:A:80:ILE:HG23	2:A:822:HOH:O	2.11	0.50
1:B:520:TYR:C	1:B:522:GLY:H	2.13	0.50
1:B:273:LEU:HB3	1:B:289:ALA:HB3	1.92	0.50
1:B:392:ARG:HH11	1:B:392:ARG:HG2	1.76	0.50
1:A:104:PHE:O	1:A:108:LEU:HB2	2.11	0.50
1:B:585:GLU:O	1:B:589:THR:HG22	2.12	0.50
1:A:64:THR:HG22	1:A:92:GLU:HG2	1.93	0.50
1:A:558:ALA:HA	1:A:618:LEU:HD13	1.94	0.50
1:A:361:LEU:O	1:A:364:GLN:HG2	2.12	0.49
1:A:743:VAL:CG1	1:A:748:ARG:HH12	2.24	0.49
1:B:646:SER:HB3	1:B:653:VAL:HG13	1.93	0.49
1:B:231:VAL:HG11	1:B:753:LEU:HD12	1.92	0.49
1:B:45:ARG:HD3	1:B:47:GLU:CG	2.43	0.49
1:A:567:PHE:N	1:A:567:PHE:CD1	2.80	0.49
1:B:558:ALA:CA	1:B:618:LEU:HD23	2.39	0.49
1:A:700:ALA:CB	1:A:717:ILE:HD13	2.41	0.49
1:A:386:HIS:HE1	1:A:640:PRO:O	1.95	0.49
1:B:532:ALA:N	1:B:533:PRO:CD	2.76	0.49
1:B:261:VAL:C	1:B:263:GLU:H	2.16	0.49
1:A:270:LEU:HA	1:A:292:ASN:HD21	1.76	0.49
1:B:293:PRO:HD3	1:B:710:HIS:HD1	1.75	0.49
1:A:753:LEU:H	1:A:753:LEU:CD2	2.25	0.49
1:B:399:THR:O	1:B:402:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:392:ARG:NH2	1:A:636:ASP:OD1	2.46	0.48
1:B:455:HIS:O	1:B:456:GLY:C	2.52	0.48
1:A:80:ILE:HG22	1:A:81:LEU:N	2.28	0.48
1:B:536:THR:HA	1:B:570:LYS:O	2.13	0.48
1:A:493:THR:N	1:A:494:PRO:CD	2.77	0.48
1:B:267:ASN:HA	1:B:706:THR:CG2	2.44	0.48
1:B:197:ILE:O	1:B:231:VAL:HA	2.14	0.48
1:A:372:PRO:O	1:A:373:ASP:HB2	2.14	0.48
1:B:498:ARG:HD2	2:B:800:HOH:O	2.13	0.48
1:A:664:GLU:CD	1:A:664:GLU:H	2.17	0.48
1:A:584:SER:H	1:A:587:GLU:HG2	1.79	0.48
1:A:674:LEU:HB3	1:A:681:PHE:HB2	1.96	0.48
1:B:609:SER:O	1:B:611:PRO:HD3	2.14	0.48
1:A:512:PHE:CE1	1:A:517:MET:HG3	2.49	0.48
1:A:498:ARG:CG	1:A:498:ARG:HH11	2.27	0.48
1:A:679:GLN:NE2	1:A:718:THR:OG1	2.45	0.48
1:A:601:GLN:HE21	1:A:601:GLN:HA	1.78	0.48
1:B:231:VAL:HG21	1:B:753:LEU:HD12	1.95	0.48
1:B:674:LEU:HB3	1:B:681:PHE:HB2	1.96	0.47
1:A:27:VAL:O	1:A:28:GLU:HG2	2.14	0.47
1:B:486:LEU:O	1:B:490:LEU:HB2	2.14	0.47
1:A:615:TRP:CE3	1:A:615:TRP:HA	2.49	0.47
1:A:169:ARG:HG2	1:A:169:ARG:H	1.56	0.47
1:A:575:ALA:O	1:A:603:VAL:HG23	2.15	0.47
1:B:99:GLY:O	1:B:103:ILE:HG13	2.14	0.47
1:A:529:GLY:C	1:A:531:THR:H	2.15	0.47
1:A:676:THR:CG2	1:A:677:TRP:N	2.77	0.47
1:B:542:ARG:HH21	1:B:629:ARG:CZ	2.28	0.47
1:A:273:LEU:HB3	1:A:289:ALA:HB3	1.96	0.47
1:B:89:LEU:HD22	1:B:98:SER:CB	2.45	0.47
1:B:68:TYR:O	1:B:87:TYR:HA	2.15	0.47
1:B:610:GLU:HB2	1:B:615:TRP:NE1	2.29	0.47
1:A:532:ALA:HB3	1:A:533:PRO:CD	2.44	0.47
1:B:268:ARG:HD2	1:B:311:LYS:HB3	1.97	0.47
1:A:458:ARG:NH2	1:A:738:ASP:OD2	2.48	0.47
1:A:569:LEU:HD21	1:A:617:ALA:HB3	1.96	0.47
1:B:657:VAL:HG22	2:B:813:HOH:O	2.15	0.47
1:A:455:HIS:ND1	1:A:455:HIS:O	2.47	0.47
1:B:258:GLU:C	1:B:260:THR:H	2.17	0.46
1:B:541:VAL:O	1:B:565:ASP:HB2	2.15	0.46
1:A:280:ALA:HB1	1:A:333:LYS:HD3	1.96	0.46
1:B:707:ASP:HA	1:B:708:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:459:GLN:HB2	1:B:459:GLN:HE21	1.53	0.46
1:B:267:ASN:HA	1:B:706:THR:HG21	1.98	0.46
1:B:563:SER:CB	1:B:626:THR:HG23	2.45	0.46
1:A:629:ARG:NH1	1:A:629:ARG:HG3	2.29	0.46
1:A:261:VAL:O	1:A:261:VAL:HG12	2.16	0.46
1:B:258:GLU:O	1:B:258:GLU:HG2	2.15	0.46
1:B:554:ILE:HG22	1:B:555:ILE:N	2.30	0.46
1:B:270:LEU:HA	1:B:292:ASN:HD21	1.80	0.46
1:B:392:ARG:HH21	1:B:636:ASP:CG	2.19	0.46
1:B:543:ALA:HA	1:B:549:THR:HG22	1.98	0.46
1:B:746:LEU:O	1:B:750:LEU:HB2	2.16	0.46
1:B:386:HIS:HE1	1:B:640:PRO:O	1.97	0.46
1:A:352:VAL:C	1:A:353:LEU:HD23	2.35	0.46
1:A:524:THR:OG1	1:A:525:SER:N	2.49	0.46
1:A:188:CYS:HA	1:A:201:CYS:HA	1.98	0.46
1:A:493:THR:HG23	1:A:724:PHE:CD2	2.51	0.46
1:A:532:ALA:HB3	1:A:533:PRO:HD3	1.97	0.46
1:B:607:GLU:OE2	1:B:624:TYR:HE2	1.97	0.45
1:A:384:SER:HB3	1:A:386:HIS:CD2	2.50	0.45
1:B:171:VAL:HG21	1:B:212:LYS:HB3	1.97	0.45
1:B:520:TYR:C	1:B:522:GLY:N	2.69	0.45
1:B:265:ALA:HB1	1:B:268:ARG:HG3	1.98	0.45
1:A:624:TYR:HB3	1:A:625:ARG:H	1.40	0.45
1:A:126:GLU:H	1:A:126:GLU:CD	2.16	0.45
1:B:134:PHE:CD1	1:B:138:LEU:HD11	2.51	0.45
1:A:152:VAL:HG13	1:A:152:VAL:O	2.17	0.45
1:B:531:THR:O	1:B:532:ALA:HB3	2.17	0.45
1:A:183:PHE:HA	1:A:189:PHE:CZ	2.51	0.45
1:B:257:THR:HG22	1:B:259:ASP:H	1.82	0.45
1:A:448:ILE:HD11	1:A:486:LEU:CD2	2.47	0.45
1:B:159:VAL:HG22	1:B:194:GLY:N	2.32	0.45
1:B:379:GLY:H	1:B:633:LYS:HG2	1.82	0.45
1:A:720:VAL:HG13	1:A:725:GLU:HA	1.99	0.45
1:A:486:LEU:O	1:A:490:LEU:HB2	2.17	0.45
1:A:134:PHE:CD1	1:A:138:LEU:HD11	2.52	0.45
1:B:324:ASN:HD22	1:B:325:MET:N	2.14	0.45
1:B:218:LYS:HB2	1:B:753:LEU:HD21	1.99	0.44
1:B:95:GLN:H	1:B:95:GLN:CD	2.20	0.44
1:A:570:LYS:HD2	1:A:571:THR:H	1.82	0.44
1:B:413:ASP:O	1:B:414:ASP:HB3	2.16	0.44
1:A:458:ARG:HG3	1:A:458:ARG:NH1	2.32	0.44
1:A:159:VAL:HG13	1:A:194:GLY:N	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:509:MET:HG2	1:B:550:ARG:HB3	1.99	0.44
1:B:569:LEU:HD22	1:B:618:LEU:HD13	1.99	0.44
1:A:584:SER:H	1:A:587:GLU:HG3	1.83	0.44
1:B:161:ARG:HG3	1:B:192:ASP:HB3	1.98	0.44
1:B:713:ARG:HB3	1:B:713:ARG:HH21	1.82	0.44
1:A:28:GLU:O	1:A:29:HIS:CB	2.64	0.44
1:A:526:ARG:O	1:A:527:GLU:C	2.55	0.44
1:A:506:ALA:HA	1:A:509:MET:HE3	1.99	0.44
1:B:654:ILE:O	1:B:654:ILE:HG13	2.17	0.44
1:A:576:TYR:CE2	1:A:614:PHE:HB2	2.53	0.44
1:A:545:SER:HB2	2:A:786:HOH:O	2.18	0.44
1:A:266:ALA:HA	1:A:652:PHE:O	2.18	0.44
1:B:625:ARG:CZ	1:B:627:SER:HB2	2.48	0.44
1:A:711:ARG:HG2	1:A:711:ARG:H	1.47	0.44
1:A:490:LEU:HA	1:A:490:LEU:HD12	1.87	0.43
1:B:455:HIS:O	1:B:458:ARG:N	2.51	0.43
1:A:504:GLU:HG2	1:A:517:MET:HE1	2.00	0.43
1:B:713:ARG:CB	1:B:713:ARG:HH21	2.31	0.43
1:A:70:ILE:HD12	1:A:70:ILE:N	2.33	0.43
1:B:293:PRO:HD3	1:B:710:HIS:CE1	2.53	0.43
1:A:262:LYS:HG3	1:A:262:LYS:O	2.18	0.43
1:B:77:ARG:CZ	1:B:378:LEU:HB3	2.48	0.43
1:A:169:ARG:HG3	1:A:655:GLU:CD	2.37	0.43
1:A:264:ASP:OD1	1:A:651:ARG:HG2	2.18	0.43
1:A:541:VAL:HG21	1:A:591:ALA:HA	2.00	0.43
1:B:753:LEU:C	1:B:755:ALA:H	2.21	0.43
1:B:507:HIS:O	1:B:511:LEU:HD13	2.19	0.43
1:B:684:VAL:O	1:B:684:VAL:CG2	2.66	0.43
1:A:353:LEU:HD23	1:A:353:LEU:N	2.33	0.43
1:A:676:THR:HG22	1:A:678:ASP:H	1.84	0.43
1:B:58:LEU:O	1:B:61:ASP:HB2	2.18	0.43
1:A:283:MET:HE1	1:A:338:PHE:HA	2.01	0.43
1:A:575:ALA:O	1:A:602:PRO:HA	2.19	0.43
1:B:314:LYS:HD3	1:B:349:GLN:HB2	1.99	0.43
1:B:27:VAL:C	1:B:29:HIS:H	2.22	0.43
1:B:374:GLN:O	1:B:633:LYS:HE2	2.19	0.43
1:A:103:ILE:O	1:A:107:GLN:HG3	2.19	0.43
1:B:228:ARG:HB3	1:B:228:ARG:NH1	2.33	0.43
1:A:321:LYS:HG2	1:A:355:GLU:OE2	2.19	0.43
1:B:164:GLN:O	1:B:173:ALA:HA	2.19	0.43
1:B:183:PHE:HA	1:B:189:PHE:CZ	2.54	0.42
1:B:633:LYS:NZ	1:B:633:LYS:HB2	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:645:CYS:SG	1:B:673:LEU:HG	2.59	0.42
1:B:277:SER:O	1:B:284:VAL:HB	2.19	0.42
1:B:218:LYS:HE3	1:B:221:ARG:HH22	1.84	0.42
1:B:324:ASN:HD22	1:B:325:MET:H	1.68	0.42
1:B:77:ARG:NH1	1:B:378:LEU:HB3	2.34	0.42
1:B:517:MET:HB2	1:B:517:MET:HE2	1.87	0.42
1:B:57:ASN:O	1:B:223:ASN:HB3	2.20	0.42
1:A:630:LEU:O	1:A:634:LYS:HB2	2.18	0.42
1:B:55:PRO:HA	1:B:56:PRO:HD3	1.91	0.42
1:A:743:VAL:CG1	1:A:748:ARG:NH1	2.82	0.42
1:A:645:CYS:HB2	1:A:671:VAL:O	2.20	0.42
1:A:207:ARG:HG3	2:A:818:HOH:O	2.18	0.42
1:A:667:ALA:HB3	1:A:670:ASP:OD2	2.19	0.42
1:A:224:GLU:C	1:A:226:SER:H	2.23	0.42
1:A:676:THR:HG21	2:A:856:HOH:O	2.19	0.42
1:B:165:VAL:HG23	1:B:171:VAL:HG13	2.01	0.42
1:B:77:ARG:NH2	1:B:378:LEU:HD13	2.35	0.42
1:B:501:GLN:HE22	1:B:521:LYS:HA	1.84	0.42
1:B:162:LEU:HD11	1:B:183:PHE:CE2	2.55	0.42
1:A:253:LEU:HA	1:A:254:PRO:HD3	1.81	0.42
1:A:118:GLN:OE1	1:A:352:VAL:HG21	2.20	0.41
1:A:506:ALA:HA	1:A:509:MET:CE	2.50	0.41
1:A:29:HIS:HA	1:A:30:PRO:HD2	1.81	0.41
1:B:161:ARG:CG	1:B:192:ASP:HB3	2.50	0.41
1:A:452:ASN:OD1	1:A:461:GLN:HG2	2.20	0.41
1:A:684:VAL:O	1:A:684:VAL:HG23	2.19	0.41
1:B:27:VAL:HG12	1:B:29:HIS:H	1.84	0.41
1:A:558:ALA:O	1:A:560:ALA:N	2.48	0.41
1:A:645:CYS:SG	1:A:673:LEU:HG	2.61	0.41
1:A:250:LYS:NZ	1:A:253:LEU:HG	2.35	0.41
1:A:332:LEU:HA	1:A:332:LEU:HD12	1.93	0.41
1:B:667:ALA:HB3	1:B:670:ASP:HB2	2.02	0.41
1:A:271:ALA:H	1:A:292:ASN:ND2	2.17	0.41
1:B:314:LYS:HD2	1:B:315:ILE:H	1.85	0.41
1:A:562:ASN:OD1	1:A:564:ASN:HB2	2.20	0.41
1:B:626:THR:O	1:B:626:THR:HG22	2.20	0.41
1:A:589:THR:HG23	1:A:590:GLY:N	2.35	0.41
1:A:617:ALA:O	1:A:618:LEU:HD23	2.21	0.41
1:B:449:ILE:HB	1:B:464:TYR:HB2	2.02	0.41
1:B:220:ILE:O	1:B:224:GLU:HB2	2.20	0.41
1:A:520:TYR:C	1:A:522:GLY:H	2.22	0.41
1:B:558:ALA:C	1:B:560:ALA:H	2.24	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:750:LEU:HA	1:B:750:LEU:HD12	1.98	0.41
1:B:138:LEU:HA	1:B:138:LEU:HD12	1.88	0.41
1:A:218:LYS:HB2	1:A:218:LYS:HE3	1.86	0.41
1:A:86:HIS:HA	1:A:119:HIS:O	2.21	0.41
1:A:85:LEU:O	1:A:119:HIS:N	2.50	0.41
1:B:347:GLN:CD	1:B:347:GLN:N	2.72	0.41
1:B:649:ILE:O	1:B:649:ILE:HG22	2.21	0.41
1:B:458:ARG:NH1	1:B:738:ASP:OD2	2.54	0.41
1:B:490:LEU:HA	1:B:490:LEU:HD12	1.85	0.41
1:B:487:ASP:OD2	1:B:492:GLY:HA2	2.20	0.41
1:A:498:ARG:CB	1:A:498:ARG:HH11	2.34	0.41
1:A:536:THR:O	1:A:556:PRO:HG2	2.21	0.41
1:A:228:ARG:HB3	1:A:228:ARG:CZ	2.50	0.41
1:B:316:PHE:CD2	1:B:316:PHE:N	2.89	0.41
1:A:204:LYS:HB3	1:A:204:LYS:HE2	1.92	0.41
1:B:281:GLY:N	1:B:282:PRO:CD	2.84	0.40
1:B:521:LYS:O	1:B:522:GLY:O	2.40	0.40
1:A:689:GLN:HG2	1:A:691:GLU:HG2	2.03	0.40
1:B:649:ILE:C	1:B:651:ARG:H	2.25	0.40
1:A:228:ARG:NH1	1:A:228:ARG:CB	2.82	0.40
1:B:127:SER:HA	1:B:349:GLN:NE2	2.37	0.40
1:B:437:THR:O	1:B:437:THR:HG22	2.21	0.40
1:B:624:TYR:HB3	1:B:625:ARG:H	1.55	0.40
1:B:52:VAL:HA	1:B:53:PRO:HD3	1.94	0.40
1:B:253:LEU:HA	1:B:254:PRO:HD3	1.79	0.40
1:B:527:GLU:O	1:B:528:GLY:C	2.59	0.40
1:A:216:VAL:O	1:A:220:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	727/729 (100%)	653 (90%)	56 (8%)	18 (2%)	9	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	727/729 (100%)	668 (92%)	41 (6%)	18 (2%)	9	12
All	All	1454/1458 (100%)	1321 (91%)	97 (7%)	36 (2%)	9	12

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ALA
1	A	367	LYS
1	A	373	ASP
1	A	456	GLY
1	A	532	ALA
1	A	624	TYR
1	B	261	VAL
1	B	264	ASP
1	B	522	GLY
1	B	527	GLU
1	B	532	ALA
1	B	625	ARG
1	A	28	GLU
1	A	266	ALA
1	A	534	ALA
1	B	280	ALA
1	B	456	GLY
1	B	632	ASP
1	A	261	VAL
1	A	526	ARG
1	A	621	LYS
1	B	263	GLU
1	B	368	ASN
1	B	526	ARG
1	B	648	LYS
1	A	29	HIS
1	A	631	LYS
1	A	650	GLY
1	B	650	GLY
1	A	556	PRO
1	A	564	ASN
1	A	622	ALA
1	B	152	VAL
1	B	154	PRO
1	B	372	PRO
1	B	528	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	597/597 (100%)	562 (94%)	35 (6%)	28	48
1	B	597/597 (100%)	558 (94%)	39 (6%)	24	42
All	All	1194/1194 (100%)	1120 (94%)	74 (6%)	26	45

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	PHE
1	A	87	TYR
1	A	96	ASP
1	A	108	LEU
1	A	162	LEU
1	A	169	ARG
1	A	170	VAL
1	A	171	VAL
1	A	193	LEU
1	A	244	LEU
1	A	246	VAL
1	A	292	ASN
1	A	307	LEU
1	A	332	LEU
1	A	347	GLN
1	A	353	LEU
1	A	385	SER
1	A	429	ASN
1	A	448	ILE
1	A	454	ARG
1	A	470	GLN
1	A	498	ARG
1	A	521	LYS
1	A	538	LEU
1	A	565	ASP
1	A	567	PHE
1	A	587	GLU
1	A	610	GLU
1	A	625	ARG

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Mol	Chain	Res	Type
1	A	657	VAL
1	A	666	LEU
1	A	674	LEU
1	A	711	ARG
1	A	721	LYS
1	A	750	LEU
1	B	49	PHE
1	B	85	LEU
1	B	138	LEU
1	B	159	VAL
1	B	162	LEU
1	B	169	ARG
1	B	193	LEU
1	B	231	VAL
1	B	246	VAL
1	B	252	THR
1	B	292	ASN
1	B	307	LEU
1	B	317	VAL
1	B	324	ASN
1	B	332	LEU
1	B	347	GLN
1	B	352	VAL
1	B	353	LEU
1	B	371	ASP
1	B	393	VAL
1	B	402	THR
1	B	459	GLN
1	B	498	ARG
1	B	499	VAL
1	B	510	SER
1	B	519	VAL
1	B	565	ASP
1	B	594	LEU
1	B	595	LEU
1	B	618	LEU
1	B	624	TYR
1	B	632	ASP
1	B	657	VAL
1	B	670	ASP
1	B	674	LEU
1	B	690	ASP

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Mol	Chain	Res	Type
1	B	694	THR
1	B	695	GLU
1	B	750	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	160	GLN
1	A	164	GLN
1	A	195	ASN
1	A	292	ASN
1	A	322	GLN
1	A	324	ASN
1	A	374	GLN
1	A	386	HIS
1	A	459	GLN
1	A	465	ASN
1	A	467	GLN
1	A	507	HIS
1	A	601	GLN
1	A	647	ASN
1	A	679	GLN
1	A	689	GLN
1	B	29	HIS
1	B	91	ASN
1	B	118	GLN
1	B	155	ASN
1	B	160	GLN
1	B	164	GLN
1	B	195	ASN
1	B	267	ASN
1	B	292	ASN
1	B	322	GLN
1	B	324	ASN
1	B	349	GLN
1	B	386	HIS
1	B	429	ASN
1	B	440	GLN
1	B	459	GLN
1	B	470	GLN
1	B	507	HIS

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Mol	Chain	Res	Type
1	B	564	ASN
1	B	601	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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, 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	729/729 (100%)	0.32	77 (10%) 7 6	14, 40, 98, 100	0
1	B	729/729 (100%)	0.21	61 (8%) 11 10	12, 37, 93, 100	0
All	All	1458/1458 (100%)	0.27	138 (9%) 8 8	12, 38, 96, 100	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	THR	9.5
1	A	532	ALA	9.1
1	A	755	ALA	9.0
1	B	261	VAL	8.7
1	A	261	VAL	8.7
1	B	279	GLY	8.6
1	A	530	GLN	8.6
1	B	378	LEU	8.6
1	A	372	PRO	8.2
1	B	373	ASP	8.0
1	B	532	ALA	7.9
1	B	259	ASP	7.7
1	B	755	ALA	7.6
1	B	530	GLN	7.6
1	B	649	ILE	7.4
1	B	531	THR	7.3
1	A	155	ASN	7.2
1	A	650	GLY	7.2
1	B	280	ALA	7.2
1	B	260	THR	7.1
1	B	377	GLY	7.0
1	A	649	ILE	7.0
1	B	265	ALA	7.0
1	B	155	ASN	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	533	PRO	6.7
1	B	374	GLN	6.6
1	A	259	ASP	6.4
1	B	264	ASP	6.0
1	B	623	THR	6.0
1	A	280	ALA	6.0
1	B	457	SER	5.9
1	A	627	SER	5.8
1	A	651	ARG	5.8
1	B	376	GLU	5.8
1	A	528	GLY	5.7
1	B	27	VAL	5.7
1	A	531	THR	5.6
1	B	262	LYS	5.6
1	A	264	ASP	5.5
1	A	265	ALA	5.5
1	B	754	ALA	5.4
1	A	622	ALA	5.4
1	A	624	TYR	5.3
1	B	156	GLU	5.1
1	A	279	GLY	4.8
1	A	573	SER	4.8
1	B	375	THR	4.6
1	A	754	ALA	4.6
1	A	457	SER	4.5
1	B	282	PRO	4.5
1	B	648	LYS	4.5
1	B	258	GLU	4.3
1	A	281	GLY	4.2
1	A	263	GLU	4.2
1	A	154	PRO	4.1
1	A	529	GLY	4.1
1	B	281	GLY	4.1
1	B	631	LYS	4.0
1	A	601	GLN	4.0
1	B	28	GLU	3.9
1	A	278	ASN	3.8
1	A	267	ASN	3.7
1	B	372	PRO	3.6
1	B	651	ARG	3.6
1	A	572	PRO	3.5
1	B	650	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	263	GLU	3.4
1	B	624	TYR	3.4
1	A	578	TRP	3.4
1	A	574	ALA	3.3
1	B	257	THR	3.3
1	A	568	VAL	3.3
1	B	154	PRO	3.2
1	A	623	THR	3.2
1	A	513	GLY	3.2
1	A	257	THR	3.2
1	A	557	LYS	3.2
1	A	153	VAL	3.2
1	A	625	ARG	3.2
1	B	380	LEU	3.2
1	A	566	ALA	3.1
1	B	370	ARG	3.1
1	B	753	LEU	3.1
1	A	567	PHE	3.0
1	A	370	ARG	3.0
1	B	278	ASN	2.9
1	B	277	SER	2.9
1	B	379	GLY	2.9
1	B	533	PRO	2.9
1	A	612	ASP	2.9
1	A	648	LYS	2.9
1	B	630	LEU	2.8
1	A	95	GLN	2.8
1	A	322	GLN	2.8
1	B	627	SER	2.8
1	B	153	VAL	2.8
1	B	306	ILE	2.8
1	A	599	ARG	2.7
1	B	228	ARG	2.7
1	A	617	ALA	2.7
1	A	605	VAL	2.7
1	B	157	VAL	2.7
1	B	616	GLU	2.7
1	A	306	ILE	2.7
1	A	581	ALA	2.6
1	A	734	LEU	2.6
1	A	555	ILE	2.6
1	A	535	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	368	ASN	2.5
1	B	321	LYS	2.5
1	A	262	LYS	2.5
1	A	258	GLU	2.5
1	A	606	ALA	2.5
1	A	538	LEU	2.5
1	B	267	ASN	2.5
1	A	569	LEU	2.5
1	A	588	LYS	2.4
1	B	528	GLY	2.4
1	B	647	ASN	2.4
1	A	579	VAL	2.3
1	A	586	ALA	2.3
1	A	576	TYR	2.3
1	A	367	LYS	2.2
1	A	454	ARG	2.2
1	B	115	ARG	2.2
1	A	156	GLU	2.2
1	A	620	GLY	2.2
1	A	735	GLY	2.2
1	A	534	ALA	2.2
1	B	734	LEU	2.1
1	B	152	VAL	2.1
1	A	282	PRO	2.1
1	A	284	VAL	2.1
1	A	436	ALA	2.1
1	A	448	ILE	2.1
1	A	302	GLU	2.1
1	B	527	GLU	2.0
1	A	583	ALA	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.