Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 09:22 pm BST

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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)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.
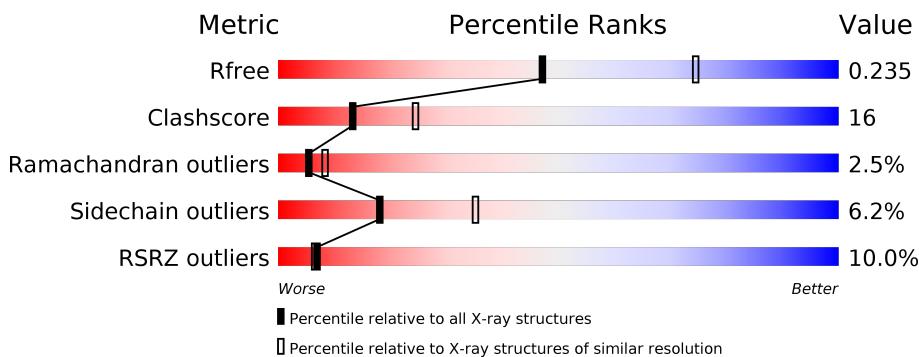
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 >=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 <=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	729	
1	B	729	
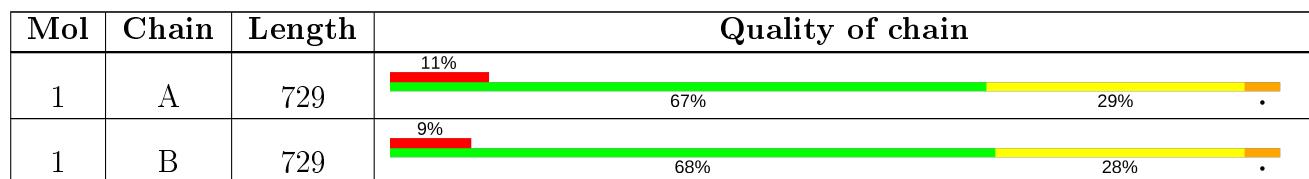
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11666 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 HORSE PLASMA GELSOLIN.

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

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total 139	O 139	0	0
2	B	145	Total 145	O 145	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 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: HORSE PLASMA GELSOLIN

• Molecule 1: HORSE PLASMA GELSOLIN
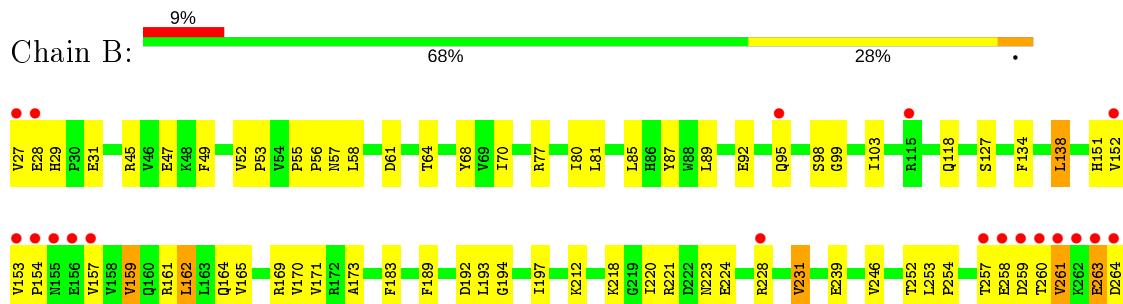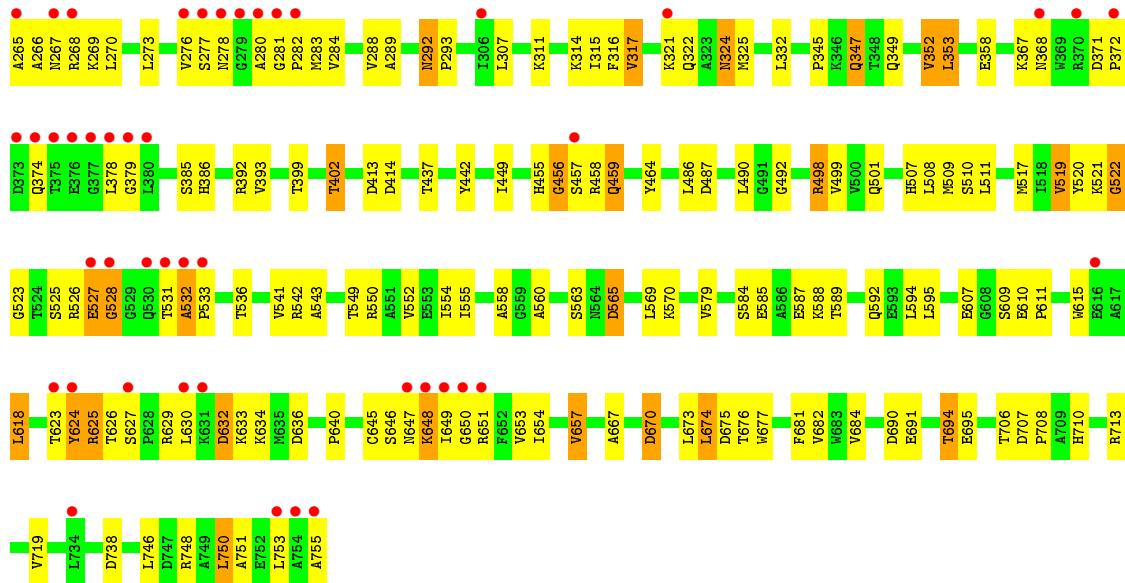
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.85 (at 2.50Å)	Xtriage
Refinement program	CNS, 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%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.3	EDS
L-test for twinning[2]	$< |L| > = 0.54, < L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11666	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 16.

All (363) 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: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:A:571:THR:HG23	1:A:573:SER:H	1.54	0.71
1:B:267:ASN:O	1:B:268:ARG:HD3	1.91	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:H	1:B:292:ASN:HD22	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:292:ASN:HD22	1:A:292:ASN:H	1.42	0.66
1:A:339:ILE:HG23	1:A:344:TYR:HB2	1.77	0.66
1:A:675:ASP:OD1	1:A:676:THR:O	2.13	0.66
1:B:170:VAL:HA	2:B:799:HOH:O	1.94	0.66
1:B:623:THR:HG22	1:B:624:TYR:H	1.61	0.66
1:A:239:GLU:CD	1:A:239:GLU:H	1.99	0.66
1:A:571:THR:OG1	1:A:572:PRO:HD2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ALA:HB2	1:A:651:ARG:HH11	1.63	0.64
1:A:585:GLU:O	1:A:589:THR:HG22	1.97	0.63
1:A:682:VAL:HG13	1:A:719:VAL:HA	1.80	0.63
1:B:151:HIS:O	1:B:153:VAL:HG23	1.98	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:A:126:GLU:HG2	1:A:131:LEU:HD21	1.82	0.61
1:B:345:PRO:HB3	1:B:347:GLN:OE1	2.00	0.61
1:A:504:GLU:HG2	1:A:517:MET:CE	2.30	0.61
1:B:347:GLN:CD	1:B:347:GLN:H	2.02	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:A:575:ALA:HB3	1:A:602:PRO:HA	1.84	0.59
1:A:626:THR:HG22	1:A:626:THR:O	2.02	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: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:H	1:B:292:ASN:ND2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:45:ARG:HD3	1:A:47:GLU:OE2	2.05	0.56
1:A:550:ARG:NH1	1:A:552:VAL:HG21	2.21	0.56
1:A:64:THR:CG2	1:A:92:GLU:HG2	2.36	0.56
1:A:414:ASP:OD2	1:A:507:HIS:HE1	1.89	0.56
1:A:753:LEU:H	1:A:753:LEU:HD22	1.71	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:509:MET:SD	1:A:550:ARG:HD3	2.46	0.55
1:A:605:VAL:HG21	1:A:610:GLU:HB3	1.88	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:228:ARG:NH1	1:A:228:ARG:HB3	2.21	0.55
1:A:662:MET:HB3	1:A:664:GLU:OE1	2.06	0.55
1:A:541:VAL:O	1:A:565:ASP:HB2	2.06	0.55
1:B:676:THR:HG22	1:B:677:TRP:N	2.20	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:152:VAL:HG22	1:A:154:PRO:HD3	1.90	0.53
1:A:279:GLY:O	1:A:280:ALA:HB2	2.08	0.53
1:A:448:ILE:HD11	1:A:486:LEU:HD23	1.90	0.53
1:A:293:PRO:HD3	1:A:710:HIS:CE1	2.43	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:276:VAL:HG13	1:B:276:VAL:O	2.09	0.52
1:B:706:THR:O	1:B:706:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:498:ARG:NH1	1:A:498:ARG:O	2.44	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: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:A:281:GLY:H	1:A:282:PRO:HD2	1.76	0.50
1:B:392:ARG:NH2	1:B:636:ASP:OD1	2.44	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:A:80:ILE:HG23	2:A:822:HOH:O	2.11	0.50
1:B:293:PRO:HG2	1:B:367:LYS:HE2	1.93	0.50
1:B:520:TYR:C	1:B:522:GLY:H	2.13	0.50
1:A:104:PHE:O	1:A:108:LEU:HB2	2.11	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: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:231:VAL:HG11	1:B:753:LEU:HD12	1.92	0.49
1:B:646:SER:HB3	1:B:653:VAL:HG13	1.93	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:A:386:HIS:HE1	1:A:640:PRO:O	1.95	0.49
1:A:700:ALA:CB	1:A:717:ILE:HD13	2.41	0.49
1:B:532:ALA:N	1:B:533:PRO:CD	2.76	0.49
1:B:558:ALA:CA	1:B:618:LEU:HD23	2.39	0.49
1:A:270:LEU:HA	1:A:292:ASN:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:VAL:C	1:B:263:GLU:H	2.16	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
1:A:392:ARG:NH2	1:A:636:ASP:OD1	2.46	0.48
1:A:80:ILE:HG22	1:A:81:LEU:N	2.28	0.48
1:B:455:HIS:O	1:B:456:GLY:C	2.52	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:A:372:PRO:O	1:A:373:ASP:HB2	2.14	0.48
1:B:197:ILE:O	1:B:231:VAL:HA	2.14	0.48
1:B:498:ARG:HD2	2:B:800:HOH:O	2.13	0.48
1:B:267:ASN:HA	1:B:706:THR:CG2	2.44	0.48
1:A:584:SER:H	1:A:587:GLU:HG2	1.79	0.48
1:A:664:GLU:CD	1:A:664:GLU:H	2.17	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:498:ARG:CG	1:A:498:ARG:HH11	2.27	0.48
1:A:512:PHE:CE1	1:A:517:MET:HG3	2.49	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:A:615:TRP:CE3	1:A:615:TRP:HA	2.49	0.47
1:B:486:LEU:O	1:B:490:LEU:HB2	2.14	0.47
1:A:169:ARG:HG2	1:A:169:ARG:H	1.56	0.47
1:A:529:GLY:C	1:A:531:THR:H	2.15	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:273:LEU:HB3	1:A:289:ALA:HB3	1.96	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:B:89:LEU:HD22	1:B:98:SER:CB	2.45	0.47
1:B:610:GLU:HB2	1:B:615:TRP:NE1	2.29	0.47
1:B:68:TYR:O	1:B:87:TYR:HA	2.15	0.47
1:A:532:ALA:HB3	1:A:533:PRO:CD	2.44	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:268:ARG:HD2	1:B:311:LYS:HB3	1.97	0.47
1:B:657:VAL:HG22	2:B:813:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:261:VAL:O	1:A:261:VAL:HG12	2.16	0.46
1:A:629:ARG:NH1	1:A:629:ARG:HG3	2.29	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:188:CYS:HA	1:A:201:CYS:HA	1.98	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:532:ALA:HB3	1:A:533:PRO:HD3	1.97	0.46
1:A:493:THR:HG23	1:A:724:PHE:CD2	2.51	0.46
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:607:GLU:OE2	1:B:624:TYR:HE2	1.97	0.45
1:B:520:TYR:C	1:B:522:GLY:N	2.69	0.45
1:A:624:TYR:HB3	1:A:625:ARG:H	1.40	0.45
1:B:265:ALA:HB1	1:B:268:ARG:HG3	1.98	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:A:720:VAL:HG13	1:A:725:GLU:HA	1.99	0.45
1:B:379:GLY:H	1:B:633:LYS:HG2	1.82	0.45
1:A:134:PHE:CD1	1:A:138:LEU:HD11	2.52	0.45
1:A:486:LEU:O	1:A:490:LEU:HB2	2.17	0.45
1:B:324:ASN:HD22	1:B:325:MET:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:159:VAL:HG13	1:A:194:GLY:N	2.33	0.44
1:A:458:ARG:NH1	1:A:458:ARG:HG3	2.32	0.44
1:B:509:MET:HG2	1:B:550:ARG:HB3	1.99	0.44
1:A:584:SER:H	1:A:587:GLU:HG3	1.83	0.44
1:B:569:LEU:HD22	1:B:618:LEU:HD13	1.99	0.44
1:B:161:ARG:HG3	1:B:192:ASP:HB3	1.98	0.44
1:A:28:GLU:O	1:A:29:HIS:CB	2.64	0.44
1:B:713:ARG:HH21	1:B:713:ARG:HB3	1.82	0.44
1:A:506:ALA:HA	1:A:509:MET:HE3	1.99	0.44
1:A:526:ARG:O	1:A:527:GLU:C	2.55	0.44
1:A:545:SER:HB2	2:A:786:HOH:O	2.18	0.44
1:A:576:TYR:CE2	1:A:614:PHE:HB2	2.53	0.44
1:B:654:ILE:O	1:B:654:ILE:HG13	2.17	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:A:70:ILE:HD12	1:A:70:ILE:N	2.33	0.43
1:B:713:ARG:CB	1:B:713:ARG:HH21	2.31	0.43
1:A:262:LYS:HG3	1:A:262:LYS:O	2.18	0.43
1:B:293:PRO:HD3	1:B:710:HIS:CE1	2.53	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:541:VAL:HG21	1:A:591:ALA:HA	2.00	0.43
1:A:264:ASP:OD1	1:A:651:ARG:HG2	2.18	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:A:103:ILE:O	1:A:107:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:ARG:HB3	1:B:228:ARG:NH1	2.33	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: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
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:A:630:LEU:O	1:A:634:LYS:HB2	2.18	0.42
1:B:57:ASN:O	1:B:223:ASN:HB3	2.20	0.42
1:B:517:MET:HB2	1:B:517:MET:HE2	1.87	0.42
1:B:55:PRO:HA	1:B:56:PRO:HD3	1.91	0.42
1:A:207:ARG:HG3	2:A:818:HOH:O	2.18	0.42
1:A:224:GLU:C	1:A:226:SER:H	2.23	0.42
1:A:667:ALA:HB3	1:A:670:ASP:OD2	2.19	0.42
1:A:645:CYS:HB2	1:A:671:VAL:O	2.20	0.42
1:A:743:VAL:CG1	1:A:748:ARG:NH1	2.82	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:A:253:LEU:HA	1:A:254:PRO:HD3	1.81	0.42
1:B:162:LEU:HD11	1:B:183:PHE:CE2	2.55	0.42
1:B:501:GLN:HE22	1:B:521:LYS:HA	1.84	0.42
1:A:29:HIS:HA	1:A:30:PRO:HD2	1.81	0.41
1:A:118:GLN:OE1	1:A:352:VAL:HG21	2.20	0.41
1:A:452:ASN:OD1	1:A:461:GLN:HG2	2.20	0.41
1:A:506:ALA:HA	1:A:509:MET:CE	2.50	0.41
1:A:684:VAL:O	1:A:684:VAL:HG23	2.19	0.41
1:B:161:ARG:CG	1:B:192:ASP:HB3	2.50	0.41
1:B:27:VAL:HG12	1:B:29:HIS:H	1.84	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:520:TYR:C	1:A:522:GLY:H	2.22	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:220:ILE:O	1:B:224:GLU:HB2	2.20	0.41
1:B:449:ILE:HB	1:B:464:TYR:HB2	2.02	0.41
1:A:218:LYS:HB2	1:A:218:LYS:HE3	1.86	0.41
1:A:85:LEU:O	1:A:119:HIS:N	2.50	0.41
1:A:86:HIS:HA	1:A:119:HIS:O	2.21	0.41
1:B:138:LEU:HA	1:B:138:LEU:HD12	1.88	0.41
1:B:558:ALA:C	1:B:560:ALA:H	2.24	0.41
1:B:750:LEU:HA	1:B:750:LEU:HD12	1.98	0.41
1:B:347:GLN:CD	1:B:347:GLN:N	2.72	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:B:649:ILE:O	1:B:649:ILE:HG22	2.21	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:204:LYS:HB3	1:A:204:LYS:HE2	1.92	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: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:A:228:ARG:CB	1:A:228:ARG:NH1	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:649:ILE:C	1:B:651:ARG:H	2.25	0.40
1:B:253:LEU:HA	1:B:254:PRO:HD3	1.79	0.40
1:B:52:VAL:HA	1:B:53:PRO:HD3	1.94	0.40
1:B:624:TYR:HB3	1:B:625:ARG:H	1.55	0.40
1:A:216:VAL:O	1:A:220:ILE:HG13	2.21	0.40
1:B:527:GLU:O	1:B:528:GLY:C	2.59	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	727/729 (100%)	653 (90%)	56 (8%)	18 (2%)	5	8
1	B	727/729 (100%)	668 (92%)	41 (6%)	18 (2%)	5	8
All	All	1454/1458 (100%)	1321 (91%)	97 (7%)	36 (2%)	5	8

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

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Mol	Chain	Res	Type
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 (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	597/597 (100%)	562 (94%)	35 (6%)	19	37
1	B	597/597 (100%)	558 (94%)	39 (6%)	17	33
All	All	1194/1194 (100%)	1120 (94%)	74 (6%)	18	35

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	B	564	ASN
1	B	601	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	729/729 (100%)	0.28	82 (11%)	5	4	14, 40, 98, 100	0
1	B	729/729 (100%)	0.18	64 (8%)	10	10	12, 37, 93, 100	0
All	All	1458/1458 (100%)	0.23	146 (10%)	7	6	12, 38, 96, 100	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	755	ALA	9.6
1	A	260	THR	9.4
1	A	532	ALA	9.3
1	B	261	VAL	9.2
1	B	279	GLY	9.2
1	B	373	ASP	9.0
1	A	261	VAL	8.7
1	B	378	LEU	8.7
1	B	755	ALA	8.5
1	A	530	GLN	8.3
1	B	530	GLN	8.1
1	A	650	GLY	8.1
1	B	531	THR	8.0
1	B	265	ALA	8.0
1	B	259	ASP	8.0
1	B	532	ALA	7.8
1	B	280	ALA	7.6
1	B	649	ILE	7.3
1	B	155	ASN	7.3
1	A	372	PRO	7.3
1	A	533	PRO	7.3
1	B	374	GLN	7.2
1	B	260	THR	7.2
1	A	155	ASN	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	377	GLY	7.0
1	A	649	ILE	6.6
1	A	531	THR	6.5
1	A	259	ASP	6.3
1	A	280	ALA	6.3
1	B	27	VAL	6.2
1	B	376	GLU	6.2
1	B	623	THR	6.0
1	B	264	ASP	5.9
1	A	528	GLY	5.9
1	A	627	SER	5.8
1	B	754	ALA	5.7
1	A	651	ARG	5.6
1	A	264	ASP	5.6
1	B	262	LYS	5.5
1	B	156	GLU	5.3
1	B	457	SER	5.3
1	A	573	SER	5.3
1	A	265	ALA	5.2
1	A	457	SER	5.2
1	A	622	ALA	5.1
1	B	258	GLU	5.0
1	B	375	THR	5.0
1	A	624	TYR	4.9
1	A	754	ALA	4.7
1	B	282	PRO	4.6
1	B	648	LYS	4.5
1	A	279	GLY	4.5
1	A	263	GLU	4.5
1	B	281	GLY	4.3
1	A	154	PRO	4.3
1	B	28	GLU	4.2
1	B	372	PRO	4.1
1	A	281	GLY	4.1
1	B	631	LYS	4.1
1	A	278	ASN	4.0
1	A	267	ASN	4.0
1	B	154	PRO	3.9
1	B	257	THR	3.9
1	A	513	GLY	3.8
1	A	529	GLY	3.7
1	B	651	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	650	GLY	3.7
1	A	257	THR	3.7
1	A	601	GLN	3.6
1	A	572	PRO	3.6
1	A	568	VAL	3.6
1	B	263	GLU	3.5
1	A	578	TRP	3.4
1	A	623	THR	3.4
1	A	574	ALA	3.4
1	A	566	ALA	3.3
1	B	624	TYR	3.3
1	B	278	ASN	3.3
1	B	153	VAL	3.3
1	A	599	ARG	3.3
1	A	95	GLN	3.2
1	A	625	ARG	3.2
1	A	153	VAL	3.2
1	A	557	LYS	3.2
1	A	567	PHE	3.2
1	B	630	LEU	3.2
1	B	627	SER	3.1
1	A	648	LYS	3.1
1	A	322	GLN	3.0
1	B	379	GLY	3.0
1	A	258	GLU	3.0
1	B	370	ARG	3.0
1	B	380	LEU	3.0
1	A	605	VAL	2.9
1	A	612	ASP	2.9
1	B	157	VAL	2.9
1	B	321	LYS	2.9
1	B	228	ARG	2.8
1	B	277	SER	2.8
1	A	617	ALA	2.8
1	A	370	ARG	2.8
1	B	306	ILE	2.8
1	B	533	PRO	2.8
1	A	306	ILE	2.7
1	A	586	ALA	2.7
1	A	538	LEU	2.7
1	B	753	LEU	2.7
1	A	569	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	616	GLU	2.6
1	A	613	SER	2.6
1	A	606	ALA	2.6
1	A	262	LYS	2.6
1	A	555	ILE	2.6
1	B	528	GLY	2.5
1	B	115	ARG	2.5
1	B	267	ASN	2.5
1	B	368	ASN	2.4
1	A	436	ALA	2.4
1	A	588	LYS	2.4
1	A	156	GLU	2.4
1	B	95	GLN	2.4
1	A	367	LYS	2.4
1	A	734	LEU	2.4
1	A	534	ALA	2.3
1	A	581	ALA	2.3
1	A	284	VAL	2.2
1	A	324	ASN	2.2
1	A	368	ASN	2.2
1	B	647	ASN	2.2
1	A	576	TYR	2.2
1	A	458	ARG	2.2
1	A	579	VAL	2.2
1	B	527	GLU	2.2
1	A	454	ARG	2.2
1	A	585	GLU	2.2
1	B	152	VAL	2.1
1	A	735	GLY	2.1
1	B	276	VAL	2.1
1	B	268	ARG	2.1
1	A	527	GLU	2.1
1	A	535	SER	2.1
1	A	448	ILE	2.1
1	A	256	ALA	2.0
1	B	734	LEU	2.0
1	A	456	GLY	2.0
1	A	620	GLY	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.