



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:13 pm BST

PDB ID : 1P8X
Title : The Calcium-Activated C-terminal half of gelsolin
Authors : Narayan, K.; Burtnick, L.D.; Robinson, R.C.
Deposited on : 2003-05-08
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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

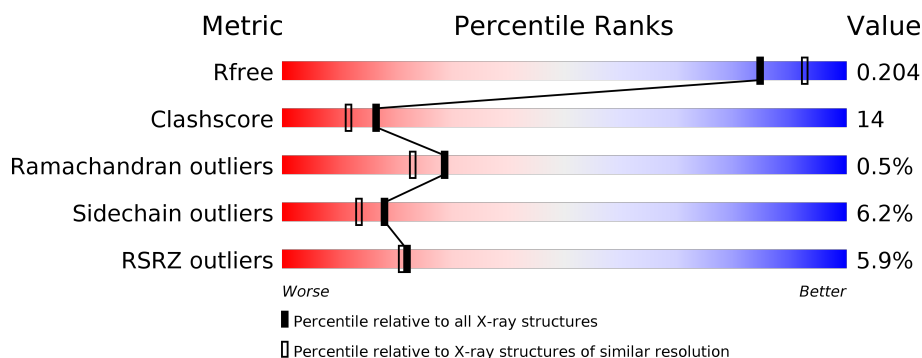
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	344	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>• 8%</div> </div> </div>
1	B	344	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 6%</div> </div> </div>
1	C	344	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>•• 6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8544 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 Gelsolin precursor, plasma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2454	1545	425	477	7			
1	B	325	Total	C	N	O	S	0	0	0
			2525	1593	436	490	6			
1	C	324	Total	C	N	O	S	0	0	0
			2516	1588	434	488	6			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	0
			3	3		

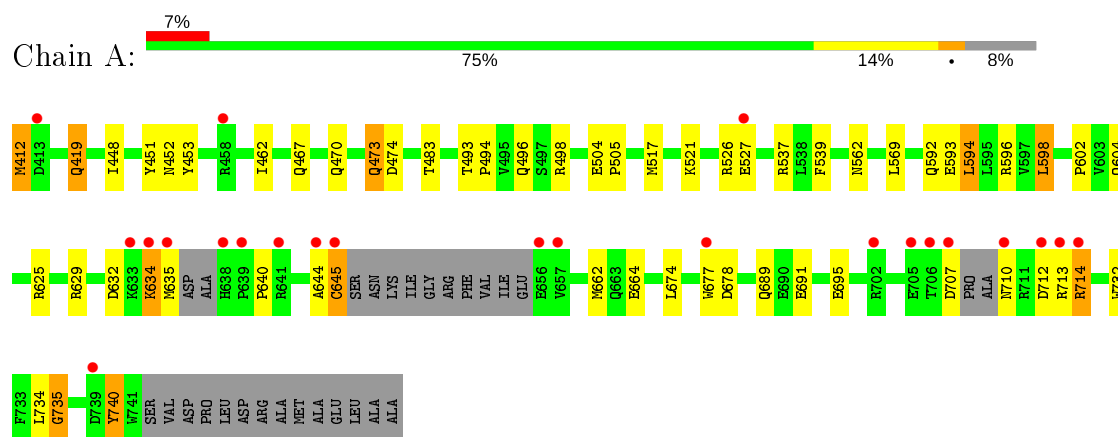
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	334	Total	O	0	0
			334	334		
3	B	374	Total	O	0	0
			374	374		
3	C	332	Total	O	0	0
			332	332		

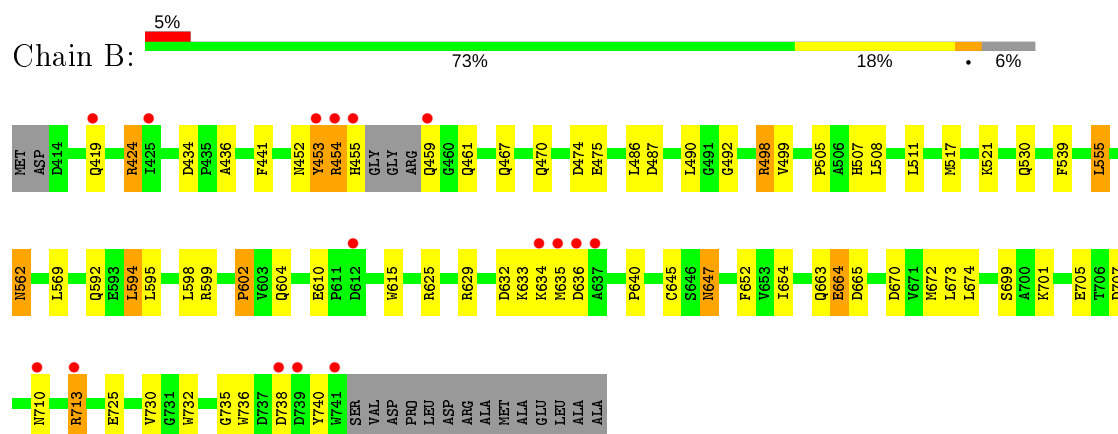
3 Residue-property plots [i](#)

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.

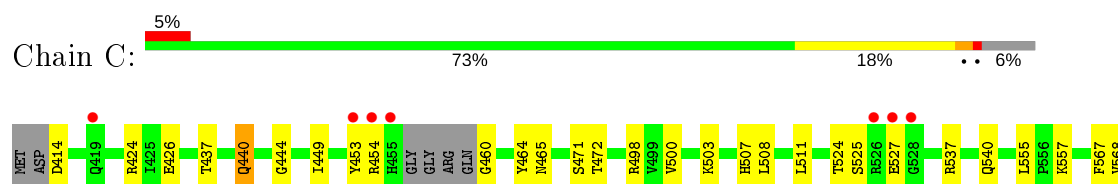
- Molecule 1: Gelsolin precursor, plasma

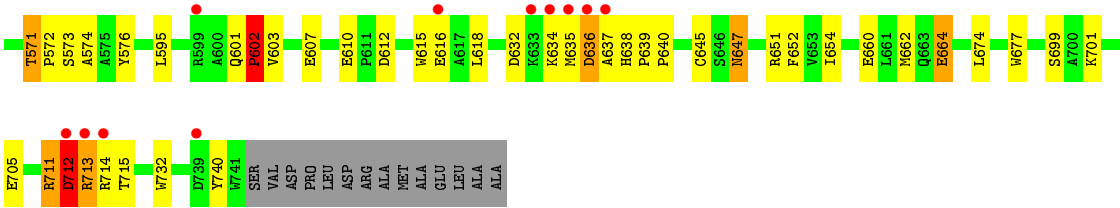


- Molecule 1: Gelsolin precursor, plasma



- Molecule 1: Gelsolin precursor, plasma





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.75Å 90.11Å 156.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 99.2 (19.96-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.85 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.245 0.206 , 0.204	Depositor DCC
R_{free} test set	4073 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8544	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.62	0/2509	0.81	0/3401
1	B	0.64	2/2584 (0.1%)	0.84	1/3508 (0.0%)
1	C	0.58	0/2575	0.79	0/3496
All	All	0.61	2/7668 (0.0%)	0.81	1/10405 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	434	ASP	CA-CB	-7.51	1.37	1.53
1	B	434	ASP	N-CA	5.87	1.58	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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	2454	0	2367	54	0
1	B	2525	0	2444	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2516	0	2434	88	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	334	0	0	11	0
3	B	374	0	0	11	1
3	C	332	0	0	18	0
All	All	8544	0	7245	209	1

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 14.

All (209) 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:C:634:LYS:NZ	1:C:636:ASP:CB	1.85	1.38
1:C:634:LYS:NZ	1:C:636:ASP:HB2	0.93	1.23
1:B:701:LYS:NZ	1:B:705:GLU:OE2	1.73	1.22
1:C:712:ASP:O	3:C:1027:HOH:O	1.60	1.15
1:B:707:ASP:OD1	1:B:710:ASN:ND2	1.84	1.11
1:C:634:LYS:HE2	1:C:636:ASP:HA	1.34	1.07
1:C:634:LYS:HZ1	1:C:636:ASP:CB	1.54	1.02
1:A:714:ARG:HD3	1:A:714:ARG:O	1.57	1.01
1:B:467:GLN:OE1	1:B:498:ARG:NH2	1.96	0.97
1:A:662:MET:CE	1:A:734:LEU:HB3	1.95	0.96
1:A:662:MET:HE2	1:A:734:LEU:HB3	1.49	0.95
1:B:707:ASP:CG	1:B:710:ASN:HD22	1.71	0.95
1:C:634:LYS:HZ3	1:C:636:ASP:CB	1.61	0.91
1:C:437:THR:O	1:C:440:GLN:HG2	1.69	0.91
1:C:634:LYS:HE2	1:C:636:ASP:CA	2.02	0.88
1:A:735:GLY:HA2	3:A:1037:HOH:O	1.73	0.88
1:B:610:GLU:OE1	3:B:1328:HOH:O	1.94	0.86
1:C:711:ARG:O	1:C:712:ASP:O	1.93	0.86
1:C:634:LYS:CE	1:C:636:ASP:HB2	2.05	0.85
1:C:634:LYS:CE	1:C:636:ASP:CB	2.56	0.83
1:B:454:ARG:O	1:B:455:HIS:HB3	1.79	0.82
1:C:571:THR:HG22	1:C:574:ALA:H	1.46	0.81
1:A:691:GLU:H	1:A:691:GLU:CD	1.81	0.80
1:C:472:THR:HG23	3:C:1119:HOH:O	1.81	0.78
1:A:412:MET:N	3:A:1336:HOH:O	2.15	0.77
1:B:713:ARG:H	1:B:713:ARG:HD3	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:LYS:CE	1:C:636:ASP:HA	2.13	0.77
1:C:571:THR:HG22	1:C:573:SER:H	1.51	0.74
1:B:707:ASP:CG	1:B:710:ASN:ND2	2.34	0.74
1:B:498:ARG:HG2	1:B:498:ARG:HH11	1.51	0.74
1:B:635:MET:O	1:B:635:MET:HG2	1.88	0.73
1:B:486:LEU:O	1:B:490:LEU:HD13	1.88	0.73
1:A:735:GLY:CA	3:A:1037:HOH:O	2.32	0.72
1:C:634:LYS:HE2	1:C:635:MET:O	1.88	0.72
1:C:634:LYS:CE	1:C:636:ASP:CA	2.67	0.72
1:C:634:LYS:HG2	1:C:635:MET:O	1.89	0.72
1:B:521:LYS:HE3	1:B:555:LEU:HD13	1.70	0.72
1:C:634:LYS:HZ3	1:C:636:ASP:HB2	0.90	0.72
1:C:677:TRP:CE2	1:C:711:ARG:HB3	2.25	0.72
1:B:664:GLU:HG2	1:B:740:TYR:OH	1.89	0.72
1:C:636:ASP:O	3:C:1184:HOH:O	2.09	0.69
1:C:571:THR:HG23	1:C:572:PRO:HD2	1.74	0.69
1:A:714:ARG:HH11	1:A:714:ARG:HG2	1.56	0.69
1:B:640:PRO:HG2	1:B:732:TRP:CE3	2.28	0.68
1:B:498:ARG:C	1:B:498:ARG:HD3	2.14	0.68
1:A:714:ARG:NH1	1:A:714:ARG:HG2	2.09	0.68
1:B:467:GLN:HB2	1:B:498:ARG:HH22	1.59	0.67
1:B:498:ARG:HG2	1:B:498:ARG:NH1	2.08	0.67
1:C:645:CYS:HB3	1:C:652:PHE:CZ	2.30	0.67
1:A:662:MET:HE1	1:A:734:LEU:HB3	1.73	0.66
1:B:610:GLU:H	1:B:610:GLU:CD	2.00	0.65
1:C:444:GLY:O	1:C:471:SER:HA	1.97	0.65
1:C:612:ASP:O	1:C:616:GLU:HG3	1.96	0.65
1:B:517:MET:HG3	3:B:1371:HOH:O	1.96	0.64
1:C:712:ASP:HB3	3:C:1274:HOH:O	1.95	0.64
1:B:713:ARG:HD3	1:B:713:ARG:N	2.13	0.63
1:A:714:ARG:CG	1:A:714:ARG:HH11	2.11	0.63
1:C:595:LEU:HD13	1:C:602:PRO:HG3	1.79	0.63
1:C:714:ARG:HG3	3:C:1039:HOH:O	1.97	0.63
1:B:610:GLU:HG3	1:B:615:TRP:CE2	2.34	0.62
1:C:634:LYS:HZ1	1:C:636:ASP:HB2	0.79	0.62
1:B:452:ASN:ND2	1:B:461:GLN:HG2	2.14	0.62
1:C:634:LYS:HZ1	1:C:636:ASP:CA	2.12	0.62
1:A:714:ARG:HA	1:A:714:ARG:HH11	1.64	0.62
1:A:712:ASP:OD1	1:A:714:ARG:N	2.26	0.62
1:B:467:GLN:HB2	1:B:498:ARG:NH2	2.15	0.61
1:C:713:ARG:HB2	3:C:1261:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ASP:OD1	1:A:710:ASN:OD1	2.19	0.60
1:C:634:LYS:NZ	1:C:636:ASP:CA	2.63	0.60
1:A:632:ASP:OD2	1:A:634:LYS:HB3	2.01	0.60
1:C:618:LEU:HB3	3:C:1314:HOH:O	2.01	0.60
1:A:517:MET:HE3	3:A:1291:HOH:O	2.01	0.60
1:C:610:GLU:HG3	1:C:615:TRP:CE2	2.36	0.59
1:B:713:ARG:H	1:B:713:ARG:CD	2.10	0.59
1:A:707:ASP:OD1	1:A:710:ASN:HA	2.03	0.58
1:C:568:VAL:HG13	1:C:595:LEU:HD21	1.84	0.58
1:A:451:TYR:CE2	1:A:453:TYR:HB3	2.38	0.58
1:C:465:ASN:CG	1:C:498:ARG:HH21	2.07	0.58
1:A:714:ARG:C	1:A:714:ARG:HD3	2.23	0.58
1:C:640:PRO:HG2	1:C:732:TRP:CE3	2.39	0.58
1:C:414:ASP:N	3:C:1334:HOH:O	2.36	0.57
1:C:576:TYR:CD1	1:C:603:VAL:CG2	2.87	0.57
1:C:714:ARG:O	1:C:715:THR:C	2.42	0.57
1:B:664:GLU:HB2	3:B:1057:HOH:O	2.05	0.57
1:A:629:ARG:NH1	1:A:677:TRP:HB3	2.20	0.56
1:C:437:THR:HB	1:C:440:GLN:HG3	1.87	0.56
1:C:576:TYR:HD1	1:C:603:VAL:CG2	2.18	0.56
1:C:636:ASP:OD1	1:C:639:PRO:HG3	2.06	0.56
1:B:629:ARG:HH12	1:B:635:MET:HB2	1.70	0.56
1:A:448:ILE:HG23	3:A:1332:HOH:O	2.05	0.55
1:C:571:THR:HG23	1:C:572:PRO:CD	2.36	0.55
1:C:677:TRP:CZ2	1:C:711:ARG:HB3	2.42	0.55
1:B:647:ASN:HD22	1:B:647:ASN:C	2.09	0.55
1:C:424:ARG:HD3	1:C:426:GLU:OE2	2.06	0.55
1:B:441:PHE:HE1	3:B:1371:HOH:O	1.90	0.55
1:B:454:ARG:CZ	1:B:455:HIS:HA	2.37	0.55
1:C:576:TYR:CD1	1:C:603:VAL:HG22	2.42	0.55
1:A:517:MET:CE	3:A:1291:HOH:O	2.53	0.54
1:C:632:ASP:OD1	1:C:634:LYS:HB3	2.08	0.54
1:A:691:GLU:N	1:A:691:GLU:OE2	2.39	0.54
1:C:637:ALA:C	1:C:639:PRO:HD3	2.28	0.54
1:B:453:TYR:CD1	1:B:459:GLN:O	2.61	0.54
1:C:414:ASP:OD2	1:C:507:HIS:HE1	1.90	0.54
1:A:594:LEU:HD22	1:A:598:LEU:HD22	1.89	0.54
1:B:595:LEU:HD13	1:B:602:PRO:HB3	1.90	0.53
1:C:464:TYR:OH	1:C:507:HIS:HD2	1.90	0.53
1:C:711:ARG:O	1:C:712:ASP:C	2.47	0.53
1:A:691:GLU:O	1:A:695:GLU:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ALA:O	1:A:645:CYS:C	2.47	0.53
1:B:604:GLN:HB3	3:B:1333:HOH:O	2.10	0.52
1:B:634:LYS:C	1:B:636:ASP:H	2.12	0.52
1:A:504:GLU:OE2	1:A:517:MET:HE3	2.10	0.52
1:A:689:GLN:HB3	1:A:691:GLU:OE2	2.10	0.52
1:C:677:TRP:NE1	1:C:711:ARG:HB3	2.25	0.51
1:C:662:MET:HE1	3:C:1104:HOH:O	2.10	0.51
1:A:640:PRO:HG2	1:A:732:TRP:CE3	2.46	0.51
1:A:634:LYS:O	1:A:635:MET:HB3	2.11	0.51
1:B:539:PHE:CG	1:B:594:LEU:HD11	2.46	0.51
1:C:440:GLN:NE2	3:C:1098:HOH:O	2.43	0.51
1:C:638:HIS:N	1:C:639:PRO:HD3	2.26	0.51
1:B:498:ARG:HD3	1:B:499:VAL:N	2.24	0.51
1:A:473:GLN:H	1:A:473:GLN:CD	2.14	0.51
1:B:454:ARG:O	1:B:455:HIS:CB	2.54	0.51
1:A:467:GLN:OE1	1:A:498:ARG:NH2	2.45	0.50
1:C:571:THR:CG2	1:C:573:SER:H	2.23	0.50
1:C:701:LYS:O	1:C:705:GLU:HG3	2.11	0.50
1:B:474:ASP:OD2	1:B:475:GLU:N	2.45	0.49
1:B:654:ILE:HD11	1:B:699:SER:OG	2.12	0.49
1:A:562:ASN:HA	1:A:625:ARG:O	2.12	0.49
1:C:601:GLN:NE2	3:C:1203:HOH:O	2.46	0.49
1:B:562:ASN:HA	1:B:625:ARG:O	2.13	0.49
1:A:498:ARG:HD2	3:A:1115:HOH:O	2.11	0.48
1:B:436:ALA:HB2	1:C:527:GLU:HB3	1.95	0.48
1:B:647:ASN:ND2	3:B:1217:HOH:O	2.46	0.48
1:C:647:ASN:C	1:C:647:ASN:HD22	2.16	0.48
1:A:412:MET:SD	1:A:462:ILE:HD11	2.53	0.48
1:A:707:ASP:HB3	1:A:710:ASN:OD1	2.13	0.48
1:A:707:ASP:CB	1:A:710:ASN:OD1	2.62	0.48
1:C:712:ASP:HB2	3:C:1260:HOH:O	2.12	0.48
1:C:715:THR:N	3:C:1274:HOH:O	2.45	0.48
1:C:571:THR:HG22	1:C:573:SER:N	2.22	0.47
1:C:610:GLU:HG3	1:C:615:TRP:CZ2	2.48	0.47
1:C:449:ILE:HB	1:C:464:TYR:HB2	1.96	0.47
1:C:634:LYS:HG2	1:C:635:MET:N	2.28	0.47
1:A:419:GLN:NE2	1:A:419:GLN:O	2.48	0.47
1:A:493:THR:N	1:A:494:PRO:HD2	2.30	0.47
1:B:508:LEU:HD12	1:B:511:LEU:HD22	1.97	0.47
1:C:713:ARG:HE	1:C:713:ARG:HA	1.81	0.46
1:B:498:ARG:C	1:B:498:ARG:CD	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:GLY:N	3:A:1037:HOH:O	2.48	0.46
1:B:663:GLN:NE2	1:B:740:TYR:HB3	2.30	0.46
1:B:424:ARG:NH2	1:B:530:GLN:OE1	2.33	0.45
1:A:483:THR:HG22	1:A:496:GLN:HE22	1.81	0.45
1:A:714:ARG:NH1	1:A:714:ARG:HA	2.30	0.45
1:A:592:GLN:NE2	3:A:1218:HOH:O	2.49	0.45
1:C:654:ILE:HD11	1:C:699:SER:OG	2.17	0.45
1:B:652:PHE:HE2	1:B:654:ILE:HD11	1.81	0.45
1:B:665:ASP:O	1:B:672:MET:HE1	2.17	0.45
1:C:555:LEU:HD23	1:C:557:LYS:HD3	1.98	0.45
1:B:629:ARG:HH22	1:B:635:MET:HG3	1.81	0.45
1:B:632:ASP:OD1	1:B:633:LYS:N	2.49	0.45
1:C:607:GLU:HG3	3:C:1303:HOH:O	2.17	0.45
1:A:419:GLN:NE2	1:A:452:ASN:HB2	2.32	0.44
1:C:701:LYS:HE3	1:C:705:GLU:OE2	2.17	0.44
1:A:629:ARG:NH1	1:A:677:TRP:CB	2.81	0.44
1:C:437:THR:HB	1:C:440:GLN:CG	2.47	0.44
1:B:735:GLY:N	3:B:1142:HOH:O	2.51	0.44
1:C:571:THR:HG22	1:C:574:ALA:N	2.26	0.44
1:B:645:CYS:HB3	1:B:652:PHE:CE1	2.53	0.44
1:C:664:GLU:OE1	1:C:664:GLU:HA	2.17	0.43
1:B:664:GLU:HG3	3:B:1304:HOH:O	2.16	0.43
1:B:645:CYS:O	1:B:670:ASP:HB3	2.17	0.43
1:C:453:TYR:C	1:C:454:ARG:HG2	2.38	0.43
1:C:524:THR:OG1	1:C:525:SER:N	2.52	0.43
1:C:607:GLU:HA	3:C:1303:HOH:O	2.17	0.43
1:A:521:LYS:HA	3:A:1134:HOH:O	2.18	0.43
1:C:500:VAL:HG22	3:C:1023:HOH:O	2.17	0.43
1:B:521:LYS:HE3	1:B:555:LEU:CD1	2.44	0.43
1:B:498:ARG:HD2	3:B:1353:HOH:O	2.18	0.42
1:B:665:ASP:O	1:B:672:MET:CE	2.66	0.42
1:C:508:LEU:O	1:C:511:LEU:HB2	2.18	0.42
1:A:419:GLN:NE2	1:A:419:GLN:C	2.73	0.42
1:A:604:GLN:HB3	3:A:1299:HOH:O	2.20	0.42
1:C:664:GLU:HG2	1:C:740:TYR:OH	2.20	0.42
1:A:593:GLU:O	1:A:596:ARG:HB3	2.20	0.42
1:B:629:ARG:HH12	1:B:635:MET:CB	2.32	0.42
1:C:440:GLN:HG3	3:C:1322:HOH:O	2.19	0.42
1:A:539:PHE:CG	1:A:594:LEU:HD11	2.54	0.41
1:B:459:GLN:HA	1:B:459:GLN:OE1	2.19	0.41
1:C:503:LYS:NZ	1:C:660:GLU:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:GLN:HG3	1:C:567:PHE:CZ	2.56	0.41
1:A:664:GLU:HB3	1:A:740:TYR:OH	2.20	0.41
1:B:474:ASP:OD2	1:B:475:GLU:HG3	2.20	0.41
1:B:507:HIS:O	1:B:511:LEU:HD13	2.21	0.41
1:B:505:PRO:HG3	3:B:1350:HOH:O	2.19	0.41
1:C:524:THR:O	1:C:525:SER:HB3	2.21	0.41
1:A:707:ASP:OD1	1:A:710:ASN:CA	2.68	0.41
1:B:592:GLN:HE21	1:B:592:GLN:HB3	1.74	0.41
1:B:730:VAL:HG13	1:B:736:TRP:CD2	2.56	0.41
1:B:735:GLY:CA	3:B:1142:HOH:O	2.69	0.41
1:A:634:LYS:HE2	1:A:634:LYS:HB3	1.86	0.40
1:C:453:TYR:HD1	1:C:460:GLY:C	2.24	0.40
1:C:647:ASN:HA	1:C:651:ARG:O	2.21	0.40
1:B:610:GLU:HG3	1:B:615:TRP:NE1	2.35	0.40
1:C:664:GLU:HB2	3:C:1123:HOH:O	2.20	0.40
1:A:689:GLN:CB	1:A:691:GLU:OE2	2.70	0.40
1:B:498:ARG:NH1	1:B:498:ARG:CG	2.75	0.40
1:B:629:ARG:HH12	1:B:635:MET:CG	2.34	0.40
1:B:487:ASP:OD2	1:B:492:GLY:HA2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:GLU:OE1	3:B:1287:HOH:O[2_574]	2.10	0.10

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	308/344 (90%)	300 (97%)	5 (2%)	3 (1%)	15 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	321/344 (93%)	313 (98%)	8 (2%)	0	100	100
1	C	320/344 (93%)	305 (95%)	13 (4%)	2 (1%)	25	19
All	All	949/1032 (92%)	918 (97%)	26 (3%)	5 (0%)	29	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	634	LYS
1	C	712	ASP
1	A	740	TYR
1	C	602	PRO
1	A	735	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	253/274 (92%)	235 (93%)	18 (7%)	14	10
1	B	261/274 (95%)	242 (93%)	19 (7%)	14	9
1	C	260/274 (95%)	249 (96%)	11 (4%)	30	27
All	All	774/822 (94%)	726 (94%)	48 (6%)	18	13

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	MET
1	A	419	GLN
1	A	470	GLN
1	A	473	GLN
1	A	474	ASP
1	A	505	PRO
1	A	526	ARG
1	A	527	GLU
1	A	537	ARG

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Mol	Chain	Res	Type
1	A	569	LEU
1	A	594	LEU
1	A	598	LEU
1	A	602	PRO
1	A	645	CYS
1	A	674	LEU
1	A	678	ASP
1	A	713	ARG
1	A	714	ARG
1	B	419	GLN
1	B	453	TYR
1	B	454	ARG
1	B	470	GLN
1	B	498	ARG
1	B	555	LEU
1	B	562	ASN
1	B	569	LEU
1	B	594	LEU
1	B	598	LEU
1	B	599	ARG
1	B	602	PRO
1	B	647	ASN
1	B	664	GLU
1	B	673	LEU
1	B	674	LEU
1	B	713	ARG
1	B	725	GLU
1	B	738	ASP
1	C	440	GLN
1	C	537	ARG
1	C	571	THR
1	C	602	PRO
1	C	636	ASP
1	C	647	ASN
1	C	664	GLU
1	C	674	LEU
1	C	711	ARG
1	C	712	ASP
1	C	713	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	A	470	GLN
1	B	419	GLN
1	B	452	ASN
1	B	461	GLN
1	B	470	GLN
1	B	485	GLN
1	B	592	GLN
1	B	604	GLN
1	B	647	ASN
1	B	710	ASN
1	C	440	GLN
1	C	452	ASN
1	C	461	GLN
1	C	470	GLN
1	C	507	HIS
1	C	592	GLN
1	C	647	ASN

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](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	316/344 (91%)	0.20	23 (7%)	15 14	16, 25, 57, 81	0
1	B	325/344 (94%)	0.10	16 (4%)	29 28	15, 26, 46, 73	0
1	C	324/344 (94%)	0.31	18 (5%)	24 23	19, 31, 51, 76	0
All	All	965/1032 (93%)	0.20	57 (5%)	22 21	15, 28, 54, 81	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	635	MET	11.6
1	A	645	CYS	8.3
1	A	635	MET	7.9
1	C	455	HIS	7.7
1	A	714	ARG	6.4
1	B	455	HIS	6.4
1	A	706	THR	6.2
1	A	710	ASN	6.1
1	B	634	LYS	5.6
1	B	454	ARG	5.5
1	C	636	ASP	5.4
1	C	453	TYR	5.2
1	A	634	LYS	5.2
1	C	633	LYS	4.9
1	C	637	ALA	4.8
1	A	713	ARG	4.8
1	B	636	ASP	4.6
1	C	527	GLU	4.6
1	A	702	ARG	4.4
1	C	454	ARG	4.3
1	A	638	HIS	4.3
1	B	459	GLN	4.2
1	B	635	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	713	ARG	4.2
1	C	599	ARG	4.0
1	B	739	ASP	3.9
1	A	705	GLU	3.9
1	C	714	ARG	3.8
1	B	453	TYR	3.8
1	C	528	GLY	3.6
1	C	712	ASP	3.5
1	C	634	LYS	3.4
1	A	413	ASP	3.1
1	A	527	GLU	3.0
1	A	656	GLU	3.0
1	B	741	TRP	2.9
1	C	713	ARG	2.8
1	A	633	LYS	2.8
1	A	639	PRO	2.7
1	B	710	ASN	2.7
1	B	637	ALA	2.7
1	A	707	ASP	2.5
1	A	712	ASP	2.5
1	A	644	ALA	2.4
1	A	458	ARG	2.4
1	A	641	ARG	2.4
1	B	612	ASP	2.3
1	C	739	ASP	2.3
1	A	657	VAL	2.3
1	A	677	TRP	2.3
1	C	526	ARG	2.3
1	C	419	GLN	2.1
1	B	419	GLN	2.1
1	B	738	ASP	2.1
1	C	616	GLU	2.1
1	A	739	ASP	2.0
1	B	425	ILE	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	C	1001	1/1	0.94	0.10	40,40,40,40	0
2	CA	B	1003	1/1	0.99	0.06	28,28,28,28	0
2	CA	A	1002	1/1	0.99	0.09	20,20,20,20	0
2	CA	A	1001	1/1	0.99	0.04	24,24,24,24	0
2	CA	C	1002	1/1	0.99	0.07	26,26,26,26	0
2	CA	B	1002	1/1	0.99	0.07	20,20,20,20	0
2	CA	A	1003	1/1	0.99	0.04	29,29,29,29	0
2	CA	C	1003	1/1	0.99	0.07	35,35,35,35	0
2	CA	B	1001	1/1	1.00	0.08	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.