



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:59 AM UTC

PDB ID : 1P8X / pdb_00001p8x
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 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
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

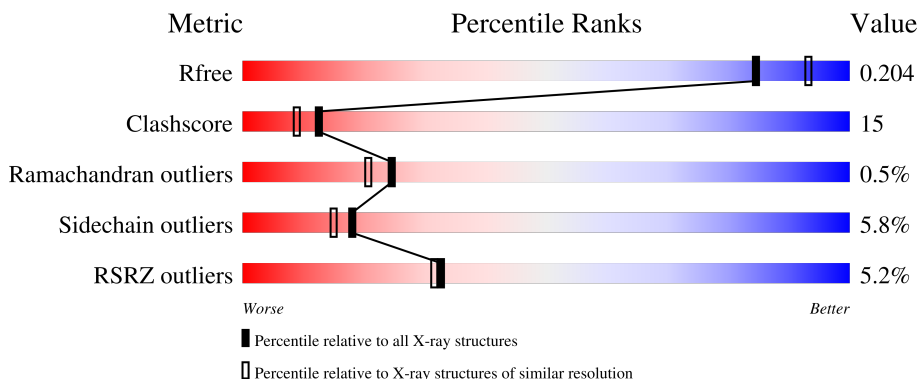
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	344	7% 74% 13% 5% 8%
1	B	344	4% 70% 19% 5% 6%
1	C	344	4% 69% 21% • 6%

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 (CCD ID: CA) (formula: Ca).

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

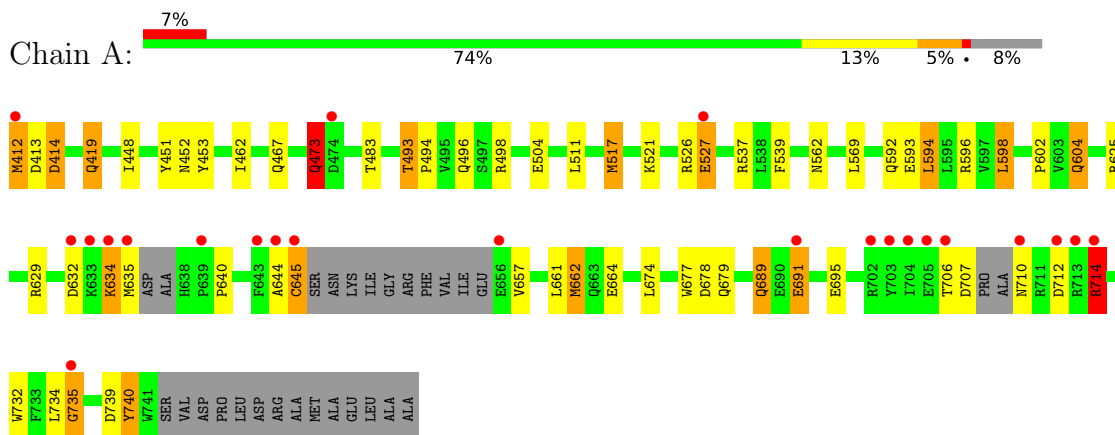
- Molecule 3 is water.

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		

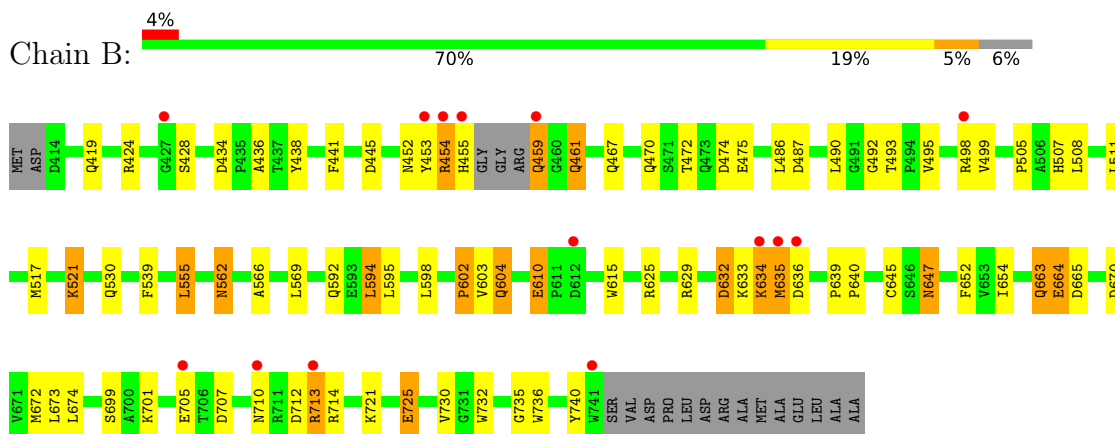
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

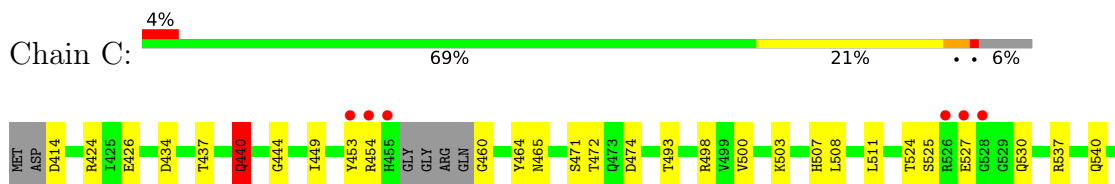
- Molecule 1: Gelsolin precursor, plasma

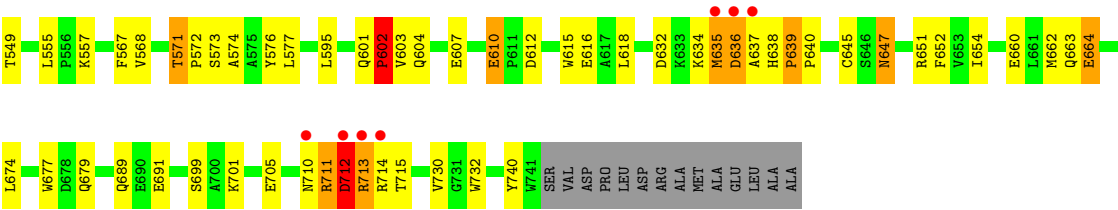


- Molecule 1: Gelsolin precursor, plasma



- 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 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 99.1 (20.00-2.00)	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 , 48.5	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 ⓘ

5.1 Standard geometry ⓘ

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	0.77	2/2509 (0.1%)	1.15	15/3401 (0.4%)
1	B	0.78	4/2584 (0.2%)	1.18	22/3508 (0.6%)
1	C	0.69	0/2575	1.17	23/3496 (0.7%)
All	All	0.75	6/7668 (0.1%)	1.17	60/10405 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	434	ASP	CA-CB	-10.13	1.37	1.53
1	B	434	ASP	N-CA	8.48	1.58	1.46
1	A	517	MET	SD-CE	-8.31	1.58	1.79
1	A	662	MET	SD-CE	-6.55	1.63	1.79
1	B	639	PRO	CA-C	5.18	1.54	1.51
1	B	434	ASP	CA-C	5.08	1.59	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	679	GLN	OE1-CD-NE2	-10.16	112.44	122.60
1	A	689	GLN	OE1-CD-NE2	-9.94	112.67	122.60
1	C	530	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	C	663	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	C	604	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	B	604	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	B	461	GLN	OE1-CD-NE2	-9.58	113.02	122.60
1	B	459	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	A	604	GLN	OE1-CD-NE2	-9.48	113.12	122.60
1	C	689	GLN	OE1-CD-NE2	-9.44	113.16	122.60
1	A	473	GLN	OE1-CD-NE2	-9.44	113.16	122.60
1	C	440	GLN	OE1-CD-NE2	-9.33	113.27	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	663	GLN	OE1-CD-NE2	-8.86	113.74	122.60
1	C	679	GLN	OE1-CD-NE2	-8.81	113.79	122.60
1	B	493	THR	CA-C-N	-7.79	112.17	120.66
1	B	493	THR	C-N-CA	-7.79	112.17	120.66
1	C	639	PRO	N-CA-C	-7.60	103.17	110.47
1	C	440	GLN	CG-CD-NE2	7.08	127.02	116.40
1	A	657	VAL	N-CA-C	7.04	113.97	107.56
1	C	604	GLN	CG-CD-NE2	7.01	126.92	116.40
1	A	689	GLN	CG-CD-NE2	7.00	126.91	116.40
1	C	679	GLN	CG-CD-NE2	6.90	126.74	116.40
1	A	679	GLN	CG-CD-NE2	6.87	126.70	116.40
1	B	604	GLN	CG-CD-NE2	6.75	126.53	116.40
1	A	604	GLN	CG-CD-NE2	6.68	126.42	116.40
1	B	428	SER	N-CA-C	-6.68	104.70	112.92
1	C	530	GLN	CG-CD-NE2	6.63	126.34	116.40
1	C	689	GLN	CG-CD-NE2	6.58	126.27	116.40
1	C	710	ASN	CA-C-N	-6.50	110.50	121.94
1	C	710	ASN	C-N-CA	-6.50	110.50	121.94
1	B	461	GLN	CG-CD-NE2	6.43	126.05	116.40
1	C	663	GLN	CG-CD-NE2	6.29	125.84	116.40
1	C	635	MET	N-CA-C	-6.25	100.59	109.96
1	B	663	GLN	CG-CD-NE2	6.18	125.67	116.40
1	A	714	ARG	N-CA-C	-6.14	104.16	112.26
1	A	414	ASP	N-CA-C	-5.99	102.45	110.24
1	A	473	GLN	CG-CD-NE2	5.95	125.33	116.40
1	B	445	ASP	N-CA-C	5.94	119.24	109.85
1	B	634	LYS	N-CA-C	-5.92	105.97	112.72
1	B	459	GLN	CG-CD-NE2	5.91	125.26	116.40
1	A	706	THR	N-CA-C	-5.87	104.80	111.14
1	B	639	PRO	N-CA-C	-5.81	104.90	110.47
1	C	712	ASP	CA-CB-CG	-5.79	106.81	112.60
1	B	632	ASP	N-CA-C	5.77	118.63	110.50
1	B	603	VAL	N-CA-C	-5.64	99.59	108.23
1	C	434	ASP	CA-C-N	5.63	126.00	119.47
1	C	434	ASP	C-N-CA	5.63	126.00	119.47
1	C	493	THR	CA-C-N	-5.59	114.50	120.03
1	C	493	THR	C-N-CA	-5.59	114.50	120.03
1	B	635	MET	N-CA-C	-5.54	105.66	113.20
1	A	493	THR	CA-C-N	-5.49	114.30	119.85
1	A	493	THR	C-N-CA	-5.49	114.30	119.85
1	C	730	VAL	N-CA-C	5.40	116.13	110.62
1	A	527	GLU	N-CA-C	5.26	117.92	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	549	THR	N-CA-C	5.21	117.89	109.40
1	B	495	VAL	N-CA-C	-5.21	102.88	109.80
1	B	521	LYS	N-CA-C	-5.20	103.53	110.55
1	B	438	TYR	CA-C-N	-5.17	117.82	123.30
1	B	438	TYR	C-N-CA	-5.17	117.82	123.30
1	B	566	ALA	N-CA-C	-5.10	101.96	110.17

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	2454	0	2367	58	0
1	B	2525	0	2444	76	0
1	C	2516	0	2434	92	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	225	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 15.

All (225) 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:A:662:MET:HE1	1:A:734:LEU:HB3	1.24	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:707:ASP:CG	1:B:710:ASN:HD22	1.71	0.99
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: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:A:691:GLU:H	1:A:691:GLU:CD	1.81	0.84
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:B:707:ASP:CG	1:B:710:ASN:ND2	2.34	0.81
1:C:571:THR:HG22	1:C:574:ALA:H	1.46	0.81
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
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: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:B:498:ARG:C	1:B:498:ARG:HD3	2.14	0.72
1:A:517:MET:HE3	3:A:1291:HOH:O	1.90	0.72
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:A:662:MET:HE1	1:A:734:LEU:CB	2.15	0.71
1:B:610:GLU:H	1:B:610:GLU:CD	2.00	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ARG:HG2	1:A:714:ARG:HH11	1.56	0.69
1:B:640:PRO:HG2	1:B:732:TRP:CE3	2.28	0.68
1:A:714:ARG:HG2	1:A:714:ARG:NH1	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: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:665:ASP:O	1:B:672:MET:HE2	1.98	0.64
1:B:713:ARG:HD3	1:B:713:ARG:N	2.13	0.63
1:A:714:ARG:HH11	1:A:714:ARG:CG	2.11	0.63
1:C:465:ASN:CG	1:C:498:ARG:HH21	2.07	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:A:714:ARG:HD3	1:A:714:ARG:C	2.23	0.62
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:HH11	1:A:714:ARG:HA	1.64	0.62
1:C:714:ARG:O	1:C:715:THR:C	2.42	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
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:B:647:ASN:HD22	1:B:647:ASN:C	2.09	0.60
1:C:618:LEU:HB3	3:C:1314: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:C:637:ALA:C	1:C:639:PRO:HD3	2.28	0.58
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:711:ARG:O	1:C:712:ASP:C	2.47	0.58
1:C:640:PRO:HG2	1:C:732:TRP:CE3	2.39	0.58
1:A:644:ALA:O	1:A:645:CYS:C	2.47	0.57
1:C:414:ASP:N	3:C:1334:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:TYR:CD1	1:C:603:VAL:CG2	2.87	0.57
1:B:634:LYS:C	1:B:636:ASP:H	2.12	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:A:504:GLU:CD	1:A:517:MET:HE1	2.31	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:473:GLN:H	1:A:473:GLN:CD	2.14	0.55
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: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:C:632:ASP:OD1	1:C:634:LYS:HB3	2.08	0.54
1:A:691:GLU:OE2	1:A:691:GLU:N	2.39	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:A:691:GLU:O	1:A:695:GLU:HG2	2.09	0.53
1:B:604:GLN:HB3	3:B:1333:HOH:O	2.10	0.52
1:C:647:ASN:C	1:C:647:ASN:HD22	2.16	0.52
1:A:689:GLN:HB3	1:A:691:GLU:OE2	2.10	0.52
1:B:498:ARG:C	1:B:498:ARG:CD	2.83	0.51
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:517:MET:CE	3:A:1291:HOH:O	2.53	0.48
1:C:453:TYR:C	1:C:454:ARG:HG2	2.38	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: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:C	2.73	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:HA	1:C:713:ARG:HE	1.81	0.46
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:C:453:TYR:HD1	1:C:460:GLY:C	2.24	0.45
1:B:652:PHE:HE2	1:B:654:ILE:HD11	1.81	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:B:647:ASN:C	1:B:647:ASN:ND2	2.75	0.44
1:A:504:GLU:OE2	1:A:517:MET:HE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:LYS:NZ	1:C:660:GLU:O	2.50	0.44
1:A:629:ARG:NH1	1:A:677:TRP:CB	2.81	0.44
1:A:661:LEU:O	1:A:662:MET:HE2	2.18	0.44
1:C:437:THR:HB	1:C:440:GLN:CG	2.47	0.44
1:B:725:GLU:H	1:B:725:GLU:CD	2.23	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:HA	1:C:664:GLU:OE1	2.17	0.43
1:B:664:GLU:HG3	3:B:1304:HOH:O	2.16	0.43
1:C:610:GLU:H	1:C:610:GLU:CD	2.25	0.43
1:B:634:LYS:C	1:B:636:ASP:N	2.77	0.43
1:B:645:CYS:O	1:B:670:ASP:HB3	2.17	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:C:691:GLU:H	1:C:691:GLU:CD	2.25	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:C:647:ASN:C	1:C:647:ASN:ND2	2.76	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:635:MET:HE2	1:B:635:MET:HB3	1.92	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:604:GLN:HB3	3:A:1299:HOH:O	2.20	0.42
1:B:712:ASP:CG	1:B:714:ARG:H	2.27	0.42
1:C:664:GLU:HG2	1:C:740:TYR:OH	2.20	0.42
1:B:454:ARG:CD	1:B:454:ARG:C	2.92	0.42
1:A:593:GLU:O	1:A:596:ARG:HB3	2.20	0.42
1:C:474:ASP:OD1	1:C:474:ASP:C	2.62	0.42
1:A:739:ASP:O	1:A:740:TYR:C	2.62	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:A:413:ASP:O	1:A:414:ASP:C	2.60	0.41
1:B:459:GLN:OE1	1:B:459:GLN:HA	2.19	0.41
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:472:THR:OG1	1:B:474:ASP:OD2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:PRO:HG3	3:B:1350:HOH:O	2.19	0.41
1:B:610:GLU:CD	1:B:610:GLU:N	2.72	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:HB3	1:A:634:LYS:HE2	1.86	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%)	12	8
1	B	321/344 (93%)	313 (98%)	8 (2%)	0	100	100
1	C	320/344 (93%)	305 (95%)	13 (4%)	2 (1%)	21	17
All	All	949/1032 (92%)	918 (97%)	26 (3%)	5 (0%)	24	21

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%)	237 (94%)	16 (6%)	16	13
1	B	261/274 (95%)	244 (94%)	17 (6%)	15	12
1	C	260/274 (95%)	248 (95%)	12 (5%)	24	22
All	All	774/822 (94%)	729 (94%)	45 (6%)	18	15

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	MET
1	A	419	GLN
1	A	473	GLN
1	A	511	LEU
1	A	526	ARG
1	A	527	GLU
1	A	537	ARG
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	691	GLU
1	A	714	ARG

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Mol	Chain	Res	Type
1	B	419	GLN
1	B	454	ARG
1	B	470	GLN
1	B	555	LEU
1	B	562	ASN
1	B	569	LEU
1	B	594	LEU
1	B	598	LEU
1	B	602	PRO
1	B	610	GLU
1	B	647	ASN
1	B	664	GLU
1	B	673	LEU
1	B	674	LEU
1	B	713	ARG
1	B	721	LYS
1	B	725	GLU
1	C	440	GLN
1	C	537	ARG
1	C	571	THR
1	C	577	LEU
1	C	602	PRO
1	C	610	GLU
1	C	636	ASP
1	C	647	ASN
1	C	664	GLU
1	C	674	LEU
1	C	711	ARG
1	C	713	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	A	440	GLN
1	A	452	ASN
1	A	455	HIS
1	B	419	GLN
1	B	421	GLN
1	B	440	GLN
1	B	452	ASN
1	B	455	HIS

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Mol	Chain	Res	Type
1	B	461	GLN
1	B	465	ASN
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	452	ASN
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 oligosaccharides 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.00	23 (7%)	21 19	16, 25, 57, 80	0
1	B	325/344 (94%)	-0.10	14 (4%)	40 39	15, 26, 46, 73	0
1	C	324/344 (94%)	0.16	13 (4%)	42 41	19, 31, 51, 76	0
All	All	965/1032 (93%)	0.02	50 (5%)	33 31	15, 28, 54, 80	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	710	ASN	5.9
1	A	635	MET	5.7
1	A	645	CYS	5.6
1	C	453	TYR	5.2
1	A	705	GLU	5.1
1	B	455	HIS	4.6
1	B	635	MET	4.5
1	A	706	THR	4.5
1	C	637	ALA	4.2
1	B	454	ARG	4.2
1	A	714	ARG	4.2
1	C	635	MET	4.1
1	B	453	TYR	4.0
1	C	636	ASP	4.0
1	C	712	ASP	3.8
1	B	710	ASN	3.5
1	C	455	HIS	3.4
1	C	454	ARG	3.4
1	A	634	LYS	3.2
1	A	527	GLU	3.0
1	C	528	GLY	3.0
1	B	459	GLN	2.9
1	A	713	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	704	ILE	2.9
1	A	412	MET	2.8
1	A	712	ASP	2.8
1	A	639	PRO	2.8
1	C	714	ARG	2.7
1	A	702	ARG	2.6
1	A	656	GLU	2.6
1	A	633	LYS	2.6
1	B	634	LYS	2.6
1	A	691	GLU	2.5
1	C	527	GLU	2.5
1	A	735	GLY	2.5
1	A	644	ALA	2.5
1	A	632	ASP	2.5
1	B	636	ASP	2.4
1	C	710	ASN	2.3
1	B	713	ARG	2.2
1	A	703	TYR	2.2
1	A	643	PHE	2.1
1	B	612	ASP	2.1
1	B	705	GLU	2.1
1	B	427	GLY	2.1
1	B	498	ARG	2.1
1	C	526	ARG	2.1
1	B	741	TRP	2.0
1	A	474	ASP	2.0
1	C	713	ARG	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](#)

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($\text{\AA}^2$)	Q<0.9
2	CA	C	1001	1/1	0.94	0.07	40,40,40,40	0
2	CA	B	1002	1/1	0.98	0.02	20,20,20,20	0
2	CA	B	1001	1/1	0.99	0.02	22,22,22,22	0
2	CA	A	1001	1/1	0.99	0.02	24,24,24,24	0
2	CA	B	1003	1/1	0.99	0.02	28,28,28,28	0
2	CA	A	1003	1/1	0.99	0.02	29,29,29,29	0
2	CA	C	1002	1/1	0.99	0.03	26,26,26,26	0
2	CA	C	1003	1/1	0.99	0.03	35,35,35,35	0
2	CA	A	1002	1/1	1.00	0.03	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.