



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:50 AM UTC

PDB ID : 3FFN / pdb_00003ffn
Title : Crystal structure of calcium-free human gelsolin
Authors : Chumnarnsilpa, S.; Robinson, R.C.; Burtnick, L.D.
Deposited on : 2008-12-04
Resolution : 3.00 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

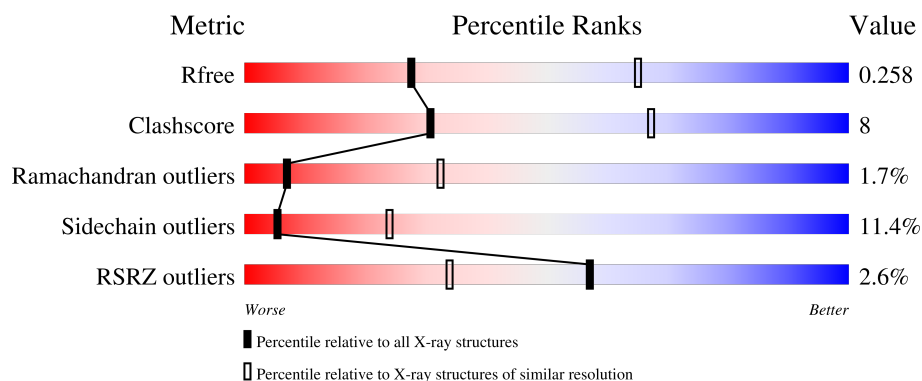
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	782	
1	B	782	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11400 atoms, of which 0 are hydrogens and 0 are deuteriums.

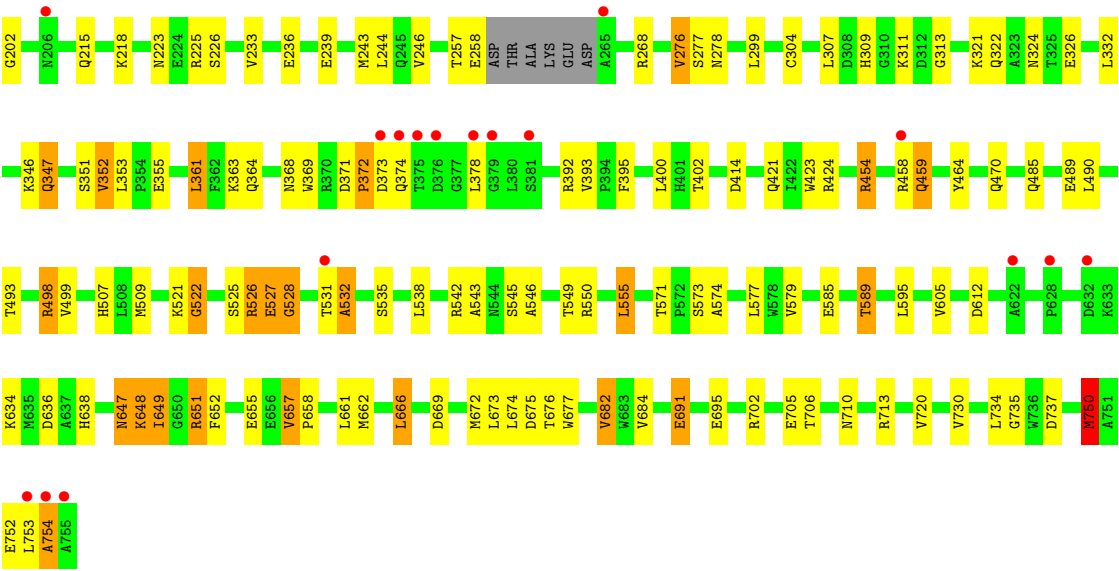
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5667	3572	991	1087	17			
1	B	723	Total	C	N	O	S	0	0	0
			5630	3551	985	1078	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	45	Total	O	0	0
			45	45		



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.89Å 170.89Å 152.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 3.00 24.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.84-3.00) 99.7 (24.84-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.58 (at 2.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.271 0.212 , 0.258	Depositor DCC
R_{free} test set	2359 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11400	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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

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	0.72	1/5796 (0.0%)	0.97	13/7852 (0.2%)
1	B	0.71	0/5759	0.96	7/7802 (0.1%)
All	All	0.72	1/11555 (0.0%)	0.96	20/15654 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	649	ILE	CA-CB	5.28	1.61	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	THR	N-CA-C	-10.12	101.70	114.56
1	A	24	SER	N-CA-C	7.13	119.13	111.36
1	A	76	LEU	N-CA-C	7.13	121.80	113.18
1	B	522	GLY	N-CA-C	6.39	128.34	113.18
1	A	371	ASP	CA-C-N	6.30	126.78	119.47
1	A	371	ASP	C-N-CA	6.30	126.78	119.47
1	B	493	THR	CA-C-N	-5.73	113.88	119.78
1	B	493	THR	C-N-CA	-5.73	113.88	119.78
1	A	27	VAL	N-CA-C	-5.72	100.34	108.58
1	A	522	GLY	N-CA-C	5.67	126.61	113.18
1	A	283	MET	N-CA-C	5.38	122.27	110.80
1	A	493	THR	CA-C-N	-5.25	114.37	119.78
1	A	493	THR	C-N-CA	-5.25	114.37	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	SER	CA-C-N	-5.22	116.72	123.19
1	B	351	SER	C-N-CA	-5.22	116.72	123.19
1	A	752	GLU	N-CA-C	5.15	116.89	111.28
1	A	374	GLN	N-CA-C	5.12	121.71	110.80
1	B	134	PHE	CA-C-N	-5.04	114.23	122.54
1	B	134	PHE	C-N-CA	-5.04	114.23	122.54
1	A	456	GLY	N-CA-C	-5.01	102.86	111.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	GLN	Peptide

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	5667	0	5516	91	0
1	B	5630	0	5483	93	0
2	A	58	0	0	1	0
2	B	45	0	0	2	0
All	All	11400	0	10999	184	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 8.

All (184) 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:A:676:THR:HG22	1:A:677:TRP:H	1.15	1.04
1:A:27:VAL:O	1:A:28:GLU:HB3	1.65	0.96
1:B:498:ARG:HG2	1:B:498:ARG:HH11	1.33	0.93
1:B:676:THR:HG22	1:B:677:TRP:H	1.35	0.91
1:B:454:ARG:HG2	1:B:454:ARG:HH11	1.40	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:O	1:A:77:ARG:HB2	1.74	0.86
1:A:498:ARG:HH11	1:A:498:ARG:HG2	1.40	0.85
1:A:676:THR:HG22	1:A:677:TRP:N	1.87	0.85
1:A:750:MET:HE3	1:A:750:MET:HA	1.59	0.85
1:B:135:LYS:HD3	1:B:662:MET:CE	2.11	0.81
1:A:364:GLN:HE21	1:A:638:HIS:HD2	1.30	0.80
1:B:750:MET:HE3	1:B:750:MET:HA	1.64	0.79
1:A:24:SER:O	1:A:25:MET:HB3	1.81	0.79
1:B:27:VAL:N	1:B:28:GLU:HA	1.97	0.78
1:B:64:THR:CG2	1:B:92:GLU:HG2	2.15	0.77
1:A:169:ARG:HD2	1:A:655:GLU:OE1	1.84	0.76
1:B:135:LYS:HD3	1:B:662:MET:HE1	1.68	0.72
1:A:364:GLN:NE2	1:A:638:HIS:HD2	1.88	0.72
1:B:498:ARG:HH11	1:B:498:ARG:CG	2.02	0.72
1:B:498:ARG:HG2	1:B:498:ARG:NH1	2.05	0.71
1:A:64:THR:CG2	1:A:92:GLU:HG2	2.20	0.71
1:B:372:PRO:O	1:B:374:GLN:N	2.19	0.70
1:A:24:SER:HB2	1:A:27:VAL:HG13	1.73	0.70
1:A:454:ARG:HH12	1:A:457:GLY:HA2	1.57	0.68
1:A:521:LYS:HE3	1:A:555:LEU:HD13	1.74	0.68
1:B:676:THR:HG22	1:B:677:TRP:N	2.07	0.68
1:A:200:TRP:CZ2	1:A:236:GLU:HG2	2.28	0.67
1:B:364:GLN:HE21	1:B:638:HIS:HD2	1.41	0.67
1:A:498:ARG:HH11	1:A:498:ARG:CG	2.06	0.67
1:A:571:THR:HG23	1:A:574:ALA:H	1.60	0.67
1:B:521:LYS:HE3	1:B:555:LEU:HD13	1.75	0.67
1:A:153:VAL:N	1:A:154:PRO:HD2	2.11	0.66
1:B:585:GLU:O	1:B:589:THR:HG22	1.94	0.66
1:A:364:GLN:HE21	1:A:638:HIS:CD2	2.12	0.66
1:B:64:THR:HG22	1:B:92:GLU:HG2	1.77	0.66
1:A:498:ARG:HG2	1:A:498:ARG:NH1	2.11	0.65
1:B:200:TRP:CZ2	1:B:236:GLU:HG2	2.31	0.65
1:B:454:ARG:HG2	1:B:454:ARG:NH1	2.10	0.64
1:B:571:THR:HG23	1:B:574:ALA:H	1.61	0.64
1:A:647:ASN:ND2	1:A:652:PHE:HD1	1.96	0.64
1:A:585:GLU:O	1:A:589:THR:HG22	1.97	0.63
1:B:647:ASN:ND2	1:B:652:PHE:HD1	1.96	0.63
1:B:29:HIS:CE1	1:B:50:ASP:OD1	2.51	0.63
1:B:268:ARG:O	1:B:309:HIS:HE1	1.82	0.61
1:B:364:GLN:NE2	1:B:638:HIS:HD2	1.98	0.60
1:A:45:ARG:HD3	1:A:47:GLU:OE2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ASP:OD1	1:A:676:THR:O	2.19	0.60
1:B:395:PHE:CD1	1:B:546:ALA:HA	2.37	0.60
1:A:29:HIS:O	1:A:32:PHE:HB3	2.02	0.59
1:B:321:LYS:HG2	1:B:355:GLU:OE2	2.03	0.59
1:A:131:LEU:HD13	1:A:170:VAL:HG12	1.84	0.59
1:B:28:GLU:N	1:B:28:GLU:CD	2.60	0.59
1:B:131:LEU:HD13	1:B:170:VAL:HG12	1.85	0.59
1:B:27:VAL:N	1:B:28:GLU:CA	2.65	0.59
1:B:675:ASP:OD1	1:B:676:THR:O	2.21	0.59
1:B:168:ARG:NH2	1:B:669:ASP:OD1	2.36	0.58
1:B:364:GLN:HE21	1:B:638:HIS:CD2	2.21	0.58
1:A:200:TRP:CD1	1:A:243:MET:HE1	2.39	0.57
1:B:200:TRP:CD1	1:B:243:MET:HE1	2.39	0.57
1:A:321:LYS:HG2	1:A:355:GLU:OE2	2.05	0.57
1:B:169:ARG:HD2	1:B:655:GLU:OE1	2.05	0.57
1:A:135:LYS:HD3	1:A:662:MET:HE1	1.87	0.57
1:B:45:ARG:HD3	1:B:47:GLU:OE2	2.05	0.56
1:A:268:ARG:O	1:A:309:HIS:HE1	1.88	0.56
1:B:421:GLN:HG2	1:B:423:TRP:CZ2	2.40	0.55
1:A:64:THR:HG22	1:A:92:GLU:HG2	1.88	0.55
1:B:61:ASP:OD1	1:B:139:LYS:NZ	2.32	0.55
1:A:50:ASP:HB2	2:A:783:HOH:O	2.05	0.55
1:A:464:TYR:OH	1:A:507:HIS:HD2	1.89	0.55
1:B:28:GLU:CD	1:B:28:GLU:H	2.15	0.55
1:B:485:GLN:O	1:B:489:GLU:HG2	2.08	0.54
1:A:191:LEU:HG	1:A:193:LEU:HD13	1.90	0.53
1:B:90:GLY:O	1:B:93:CYS:HB2	2.08	0.53
1:A:454:ARG:HG3	1:A:459:GLN:NE2	2.24	0.53
1:B:392:ARG:NH2	1:B:636:ASP:OD2	2.39	0.53
1:B:313:GLY:HA2	2:B:768:HOH:O	2.08	0.52
1:B:459:GLN:HE21	1:B:459:GLN:N	2.06	0.52
1:A:135:LYS:HD3	1:A:662:MET:CE	2.39	0.52
1:A:454:ARG:NH1	1:A:457:GLY:HA2	2.23	0.52
1:A:264:ASP:O	1:A:653:VAL:HG23	2.10	0.52
1:B:648:LYS:O	1:B:649:ILE:HB	2.08	0.52
1:B:218:LYS:HD2	1:B:753:LEU:O	2.09	0.52
1:A:90:GLY:O	1:A:93:CYS:HB2	2.11	0.51
1:A:425:ILE:HG13	1:A:479:SER:HB3	1.93	0.51
1:A:424:ARG:NH1	1:A:525:SER:OG	2.42	0.51
1:A:440:GLN:NE2	1:A:520:TYR:OH	2.43	0.51
1:B:191:LEU:HG	1:B:193:LEU:HD13	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:ALA:HB2	1:B:549:THR:HG22	1.92	0.50
1:A:118:GLN:HB2	1:A:352:VAL:HG22	1.92	0.50
1:A:347:GLN:H	1:A:347:GLN:CD	2.19	0.50
1:A:750:MET:HA	1:A:750:MET:CE	2.35	0.50
1:B:361:LEU:HD11	2:B:756:HOH:O	2.11	0.50
1:B:470:GLN:NE2	1:B:522:GLY:HA3	2.26	0.50
1:B:509:MET:HE2	1:B:550:ARG:HD3	1.94	0.49
1:A:705:GLU:HG2	1:A:713:ARG:HH11	1.77	0.49
1:B:666:LEU:HD12	1:B:672:MET:HG3	1.94	0.49
1:B:372:PRO:C	1:B:374:GLN:H	2.16	0.49
1:B:392:ARG:HH21	1:B:636:ASP:CG	2.21	0.49
1:B:705:GLU:HG2	1:B:713:ARG:HH11	1.77	0.48
1:B:647:ASN:ND2	1:B:652:PHE:CD1	2.79	0.48
1:B:400:LEU:C	1:B:402:THR:H	2.22	0.48
1:A:24:SER:HB2	1:A:27:VAL:CG1	2.43	0.48
1:A:734:LEU:HD12	1:A:735:GLY:H	1.79	0.48
1:A:648:LYS:O	1:A:649:ILE:HB	2.13	0.48
1:A:324:ASN:ND2	1:A:326:GLU:HB2	2.29	0.47
1:A:536:THR:HA	1:A:570:LYS:O	2.14	0.47
1:B:691:GLU:O	1:B:695:GLU:HG2	2.14	0.47
1:A:139:LYS:HG2	1:A:173:ALA:HB3	1.97	0.47
1:B:657:VAL:HA	1:B:658:PRO:HD3	1.77	0.47
1:B:464:TYR:OH	1:B:507:HIS:HD2	1.98	0.46
1:B:29:HIS:HE1	1:B:50:ASP:OD1	1.98	0.46
1:A:454:ARG:NH1	1:A:456:GLY:O	2.49	0.46
1:A:485:GLN:O	1:A:489:GLU:HG2	2.15	0.46
1:A:691:GLU:O	1:A:695:GLU:HG2	2.16	0.46
1:A:543:ALA:HB2	1:A:549:THR:HG22	1.97	0.46
1:B:750:MET:HA	1:B:750:MET:CE	2.40	0.46
1:B:648:LYS:HE3	1:B:649:ILE:H	1.81	0.46
1:B:118:GLN:HB2	1:B:352:VAL:HG22	1.96	0.46
1:B:225:ARG:O	1:B:226:SER:C	2.59	0.45
1:A:43:ILE:HD12	1:A:59:TYR:CG	2.52	0.45
1:A:185:ASN:O	1:A:202:GLY:HA3	2.17	0.45
1:B:392:ARG:NH2	1:B:636:ASP:CG	2.74	0.45
1:A:57:ASN:HD21	1:A:153:VAL:HG21	1.81	0.45
1:A:647:ASN:ND2	1:A:652:PHE:CD1	2.81	0.45
1:A:24:SER:O	1:A:25:MET:CB	2.58	0.45
1:B:324:ASN:ND2	1:B:326:GLU:HB2	2.32	0.45
1:B:347:GLN:H	1:B:347:GLN:CD	2.25	0.45
1:B:750:MET:O	1:B:754:ALA:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASN:N	1:B:80:ASN:HD22	2.15	0.45
1:B:139:LYS:HG2	1:B:173:ALA:HB3	1.98	0.45
1:B:454:ARG:NH1	1:B:454:ARG:CG	2.79	0.45
1:A:509:MET:HE2	1:A:550:ARG:HD3	1.99	0.44
1:B:89:LEU:HD22	1:B:98:SER:CB	2.48	0.44
1:A:470:GLN:NE2	1:A:522:GLY:HA3	2.32	0.44
1:B:185:ASN:O	1:B:202:GLY:HA3	2.18	0.44
1:B:395:PHE:CE1	1:B:546:ALA:HA	2.52	0.44
1:B:702:ARG:O	1:B:706:THR:HG23	2.18	0.44
1:A:400:LEU:C	1:A:402:THR:H	2.26	0.44
1:A:162:LEU:HD11	1:A:183:PHE:CE2	2.53	0.44
1:B:85:LEU:HD21	1:B:108:LEU:HD13	1.99	0.44
1:B:651:ARG:HE	1:B:651:ARG:HB2	1.63	0.43
1:B:233:VAL:HG11	1:B:750:MET:HE2	1.99	0.43
1:A:233:VAL:HG11	1:A:750:MET:HE2	2.01	0.43
1:B:424:ARG:NH1	1:B:525:SER:OG	2.50	0.43
1:A:464:TYR:OH	1:A:507:HIS:CD2	2.71	0.43
1:A:31:GLU:CG	1:A:44:TRP:HE1	2.32	0.43
1:A:64:THR:HG23	1:A:92:GLU:HG2	2.00	0.43
1:A:64:THR:HB	1:A:141:LYS:O	2.19	0.43
1:B:527:GLU:O	1:B:528:GLY:C	2.62	0.43
1:B:673:LEU:HD23	1:B:682:VAL:HB	2.01	0.43
1:A:27:VAL:O	1:A:28:GLU:CB	2.47	0.43
1:A:527:GLU:O	1:A:528:GLY:C	2.62	0.42
1:B:64:THR:HG23	1:B:92:GLU:HG2	1.98	0.42
1:B:414:ASP:OD2	1:B:507:HIS:HE1	2.02	0.42
1:A:657:VAL:HA	1:A:658:PRO:HD3	1.73	0.42
1:A:131:LEU:HD13	1:A:170:VAL:CG1	2.50	0.42
1:B:526:ARG:HE	1:B:526:ARG:HB3	1.66	0.42
1:A:36:GLY:O	1:A:83:TYR:OH	2.31	0.42
1:A:185:ASN:ND2	1:A:236:GLU:OE1	2.51	0.42
1:A:698:THR:HG22	1:A:702:ARG:HE	1.85	0.42
1:B:117:VAL:HG13	1:B:353:LEU:HD23	2.02	0.42
1:B:402:THR:HG22	1:B:402:THR:O	2.17	0.42
1:A:283:MET:HE3	1:A:283:MET:HB3	1.83	0.42
1:B:57:ASN:O	1:B:223:ASN:HB3	2.20	0.42
1:A:526:ARG:O	1:A:527:GLU:C	2.62	0.42
1:A:648:LYS:HE3	1:A:649:ILE:H	1.85	0.42
1:B:276:VAL:HG22	1:B:304:CYS:HB2	2.01	0.42
1:A:361:LEU:HD12	1:A:361:LEU:H	1.85	0.41
1:B:459:GLN:HE21	1:B:459:GLN:H	1.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:THR:O	1:B:532:ALA:HB3	2.20	0.41
1:A:425:ILE:HG13	1:A:479:SER:CB	2.51	0.41
1:B:215:GLN:HE21	1:B:215:GLN:HB2	1.75	0.41
1:A:57:ASN:O	1:A:223:ASN:HB3	2.21	0.41
1:A:323:ALA:O	1:A:328:ARG:NH1	2.54	0.41
1:B:64:THR:HB	1:B:141:LYS:O	2.20	0.41
1:B:734:LEU:HD12	1:B:735:GLY:H	1.86	0.41
1:B:363:LYS:HD2	1:B:369:TRP:CD1	2.56	0.41
1:A:176:VAL:HB	1:A:177:PRO:HD2	2.02	0.41
1:A:702:ARG:O	1:A:706:THR:HG23	2.21	0.41
1:A:283:MET:HG3	1:A:337:ASP:HB2	2.02	0.41
1:A:676:THR:CG2	1:A:677:TRP:N	2.62	0.40
1:A:307:LEU:HD12	1:A:307:LEU:C	2.46	0.40
1:A:380:LEU:HB3	1:A:381:SER:H	1.72	0.40
1:A:682:VAL:HG13	1:A:719:VAL:HG22	2.03	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	724/782 (93%)	673 (93%)	37 (5%)	14 (2%)	6	30
1	B	719/782 (92%)	670 (93%)	38 (5%)	11 (2%)	8	35
All	All	1443/1564 (92%)	1343 (93%)	75 (5%)	25 (2%)	7	32

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	649	ILE
1	A	751	ALA
1	B	373	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	649	ILE
1	A	25	MET
1	A	28	GLU
1	A	77	ARG
1	A	154	PRO
1	A	528	GLY
1	B	372	PRO
1	B	528	GLY
1	B	752	GLU
1	A	374	GLN
1	A	573	SER
1	B	368	ASN
1	B	545	SER
1	B	750	MET
1	A	265	ALA
1	A	368	ASN
1	A	754	ALA
1	B	532	ALA
1	B	573	SER
1	B	754	ALA
1	A	750	MET
1	A	278	ASN

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	593/630 (94%)	525 (88%)	68 (12%)	5	24
1	B	588/630 (93%)	521 (89%)	67 (11%)	5	24
All	All	1181/1260 (94%)	1046 (89%)	135 (11%)	5	24

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	27	VAL
1	A	28	GLU
1	A	33	LEU
1	A	48	LYS
1	A	49	PHE
1	A	64	THR
1	A	126	GLU
1	A	136	SER
1	A	139	LYS
1	A	152	VAL
1	A	159	VAL
1	A	162	LEU
1	A	169	ARG
1	A	171	VAL
1	A	193	LEU
1	A	239	GLU
1	A	244	LEU
1	A	246	VAL
1	A	276	VAL
1	A	283	MET
1	A	299	LEU
1	A	307	LEU
1	A	311	LYS
1	A	322	GLN
1	A	332	LEU
1	A	346	LYS
1	A	347	GLN
1	A	351	SER
1	A	352	VAL
1	A	361	LEU
1	A	371	ASP
1	A	373	ASP
1	A	374	GLN
1	A	375	THR
1	A	378	LEU
1	A	393	VAL
1	A	421	GLN
1	A	458	ARG
1	A	490	LEU
1	A	498	ARG
1	A	499	VAL
1	A	535	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	536	THR
1	A	538	LEU
1	A	542	ARG
1	A	555	LEU
1	A	577	LEU
1	A	579	VAL
1	A	587	GLU
1	A	589	THR
1	A	595	LEU
1	A	605	VAL
1	A	612	ASP
1	A	634	LYS
1	A	647	ASN
1	A	648	LYS
1	A	657	VAL
1	A	661	LEU
1	A	666	LEU
1	A	674	LEU
1	A	682	VAL
1	A	684	VAL
1	A	691	GLU
1	A	710	ASN
1	A	720	VAL
1	A	730	VAL
1	A	737	ASP
1	B	28	GLU
1	B	29	HIS
1	B	34	LYS
1	B	48	LYS
1	B	64	THR
1	B	136	SER
1	B	139	LYS
1	B	157	VAL
1	B	159	VAL
1	B	162	LEU
1	B	169	ARG
1	B	171	VAL
1	B	193	LEU
1	B	239	GLU
1	B	244	LEU
1	B	246	VAL
1	B	257	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	258	GLU
1	B	276	VAL
1	B	277	SER
1	B	278	ASN
1	B	299	LEU
1	B	307	LEU
1	B	311	LYS
1	B	322	GLN
1	B	332	LEU
1	B	346	LYS
1	B	347	GLN
1	B	352	VAL
1	B	361	LEU
1	B	371	ASP
1	B	378	LEU
1	B	393	VAL
1	B	454	ARG
1	B	458	ARG
1	B	459	GLN
1	B	490	LEU
1	B	498	ARG
1	B	499	VAL
1	B	526	ARG
1	B	527	GLU
1	B	535	SER
1	B	538	LEU
1	B	542	ARG
1	B	555	LEU
1	B	577	LEU
1	B	579	VAL
1	B	589	THR
1	B	595	LEU
1	B	605	VAL
1	B	612	ASP
1	B	634	LYS
1	B	647	ASN
1	B	648	LYS
1	B	651	ARG
1	B	657	VAL
1	B	661	LEU
1	B	666	LEU
1	B	674	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	682	VAL
1	B	684	VAL
1	B	691	GLU
1	B	710	ASN
1	B	720	VAL
1	B	730	VAL
1	B	737	ASP
1	B	750	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	91	ASN
1	A	155	ASN
1	A	164	GLN
1	A	198	HIS
1	A	215	GLN
1	A	309	HIS
1	A	364	GLN
1	A	440	GLN
1	A	461	GLN
1	A	465	ASN
1	A	467	GLN
1	A	470	GLN
1	A	507	HIS
1	A	564	ASN
1	A	638	HIS
1	A	647	ASN
1	A	679	GLN
1	B	78	ASN
1	B	80	ASN
1	B	91	ASN
1	B	164	GLN
1	B	185	ASN
1	B	198	HIS
1	B	278	ASN
1	B	309	HIS
1	B	440	GLN
1	B	459	GLN
1	B	461	GLN
1	B	470	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	507	HIS
1	B	564	ASN
1	B	638	HIS
1	B	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](#)

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 ⓘ

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	728/782 (93%)	-0.03	20 (2%) 56 33	21, 44, 79, 97	0
1	B	723/782 (92%)	0.01	18 (2%) 58 35	21, 44, 83, 97	0
All	All	1451/1564 (92%)	-0.01	38 (2%) 57 34	21, 44, 81, 97	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	ASP	6.8
1	B	381	SER	5.2
1	B	753	LEU	4.9
1	B	265	ALA	4.7
1	B	27	VAL	4.1
1	A	376	ASP	4.0
1	B	379	GLY	3.9
1	B	754	ALA	3.6
1	A	753	LEU	3.4
1	B	375	THR	3.3
1	A	280	ALA	3.1
1	A	755	ALA	2.9
1	A	754	ALA	2.9
1	A	155	ASN	2.9
1	B	628	PRO	2.9
1	A	157	VAL	2.7
1	A	265	ALA	2.6
1	A	153	VAL	2.6
1	A	152	VAL	2.5
1	A	156	GLU	2.5
1	A	154	PRO	2.4
1	B	531	THR	2.4
1	A	279	GLY	2.4
1	B	458	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	649	ILE	2.3
1	B	755	ALA	2.3
1	B	622	ALA	2.2
1	A	603	VAL	2.2
1	B	632	ASP	2.2
1	B	378	LEU	2.2
1	A	605	VAL	2.2
1	B	374	GLN	2.2
1	A	266	ALA	2.2
1	B	373	ASP	2.2
1	A	375	THR	2.1
1	A	379	GLY	2.1
1	B	206	ASN	2.0
1	A	611	PRO	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 oligosaccharides 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.