



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:53 pm BST

PDB ID : 3FFN
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 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

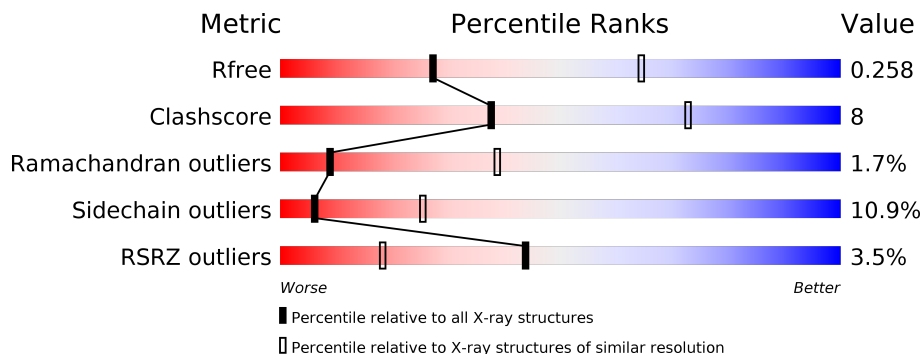
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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	782	 3% 72% 18% • 7%
1	B	782	 4% 71% 18% • 8%

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.

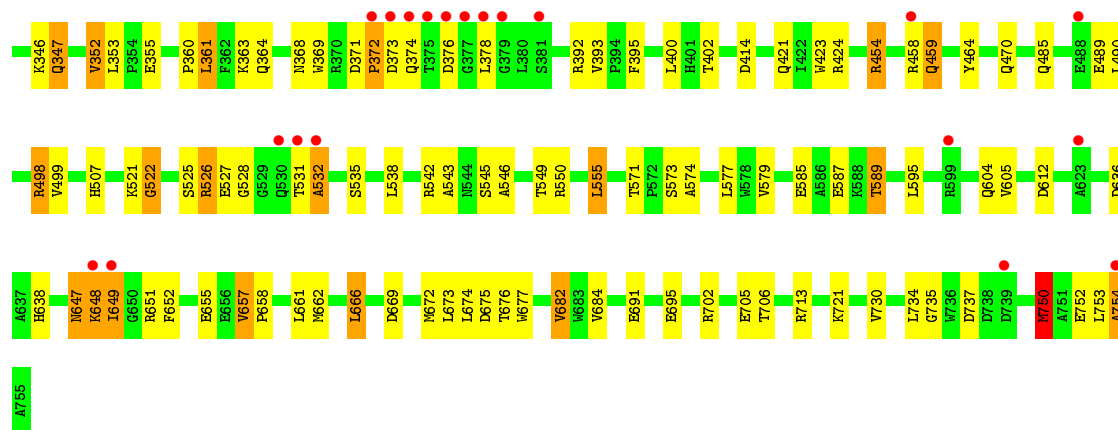
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gelsolin.

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

- 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 24.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.84-3.00) 99.9 (24.83-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.58 (at 2.99Å)	Xtrriage
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	Xtrriage
Anisotropy	0.004	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.59	0/5796	0.69	2/7852 (0.0%)
1	B	0.58	0/5759	0.68	3/7802 (0.0%)
All	All	0.59	0/11555	0.69	5/15654 (0.0%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	522	GLY	N-CA-C	6.09	128.34	113.10
1	A	522	GLY	N-CA-C	5.41	126.61	113.10
1	B	307	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	376	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	376	ASP	CB-CG-OD2	5.19	122.97	118.30

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 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	5667	0	5516	83	0
1	B	5630	0	5483	88	0
2	A	58	0	0	1	0
2	B	45	0	0	2	0
All	All	11400	0	10999	171	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 (171) 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
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: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: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:A:364:GLN:NE2	1:A:638:HIS:HD2	1.88	0.72
1:B:498:ARG:CG	1:B:498:ARG:HH11	2.02	0.72
1:B:498:ARG:NH1	1:B:498:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:135:LYS:HD3	1:B:662:MET:HE1	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:NH1	1:A:498:ARG:HG2	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
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: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:750:MET:HA	1:A:750:MET:CE	2.35	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: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:464:TYR:OH	1:A:507:HIS:HD2	1.89	0.55
1:A:50:ASP:HB2	2:A:783:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:N	1:B:28:GLU:CD	2.60	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:648:LYS:O	1:B:649:ILE:HB	2.08	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:N	1:B:459:GLN:HE21	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: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:B:750:MET:HA	1:B:750:MET:CE	2.40	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
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:B:28:GLU:H	1:B:28:GLU:CD	2.15	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: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: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: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: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:324:ASN:ND2	1:A:326:GLU:HB2	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ALA:HB2	1:A:549:THR:HG22	1.97	0.46
1:B:648:LYS:HE3	1:B:649:ILE:H	1.81	0.46
1:A:347:GLN:CD	1:A:347:GLN:H	2.19	0.46
1:B:118:GLN:HB2	1:B:352:VAL:HG22	1.96	0.46
1:A:185:ASN:O	1:A:202:GLY:HA3	2.17	0.45
1:A:43:ILE:HD12	1:A:59:TYR:CG	2.52	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:750:MET:O	1:B:754:ALA:HB3	2.17	0.45
1:B:139:LYS:HG2	1:B:173:ALA:HB3	1.98	0.45
1:B:80:ASN:N	1:B:80:ASN:HD22	2.15	0.45
1:A:61:ASP:OD1	1:A:139:LYS:NZ	2.44	0.45
1:B:454:ARG:NH1	1:B:454:ARG:CG	2.79	0.45
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:372:PRO:C	1:B:374:GLN:H	2.16	0.44
1:B:392:ARG:HH21	1:B:636:ASP:CG	2.21	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: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:400:LEU:C	1:B:402:THR:H	2.22	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: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: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:HB3	1:B:526:ARG:HE	1.66	0.42
1:A:185:ASN:ND2	1:A:236:GLU:OE1	2.51	0.42
1:A:36:GLY:O	1:A:83:TYR:OH	2.31	0.42
1:A:698:THR:HG22	1:A:702:ARG:HE	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:VAL:HG13	1:B:353:LEU:HD23	2.02	0.42
1:B:402:THR:O	1:B:402:THR:HG22	2.17	0.42
1:B:57:ASN:O	1:B:223:ASN:HB3	2.20	0.42
1:A:648:LYS:HE3	1:A:649:ILE:H	1.85	0.42
1:A:750:MET:HA	1:A:750:MET:HE3	2.01	0.42
1:B:276:VAL:HG22	1:B:304:CYS:HB2	2.01	0.42
1:A:361:LEU:H	1:A:361:LEU:HD12	1.85	0.41
1:B:459:GLN:H	1:B:459:GLN:HE21	1.66	0.41
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:HB2	1:B:215:GLN:HE21	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:B:225:ARG:O	1:B:226:SER:C	2.59	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:B:392:ARG:NH2	1:B:636:ASP:CG	2.74	0.40
1:A:380:LEU:HB3	1:A:381:SER:H	1.72	0.40
1:B:347:GLN:CD	1:B:347:GLN:H	2.25	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 [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	724/782 (93%)	673 (93%)	37 (5%)	14 (2%)	8 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	719/782 (92%)	670 (93%)	38 (5%)	11 (2%)	10	42
All	All	1443/1564 (92%)	1343 (93%)	75 (5%)	25 (2%)	9	39

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	649	ILE
1	A	751	ALA
1	B	373	ASP
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 [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	593/630 (94%)	527 (89%)	66 (11%)	6	25
1	B	588/630 (93%)	525 (89%)	63 (11%)	6	26
All	All	1181/1260 (94%)	1052 (89%)	129 (11%)	6	25

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	27	VAL
1	A	28	GLU
1	A	33	LEU
1	A	49	PHE
1	A	64	THR
1	A	93	CYS
1	A	136	SER
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	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	393	VAL
1	A	421	GLN
1	A	458	ARG

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Mol	Chain	Res	Type
1	A	465	ASN
1	A	490	LEU
1	A	498	ARG
1	A	499	VAL
1	A	535	SER
1	A	538	LEU
1	A	542	ARG
1	A	550	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	604	GLN
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	721	LYS
1	A	730	VAL
1	A	737	ASP
1	A	750	MET
1	B	29	HIS
1	B	34	LYS
1	B	49	PHE
1	B	64	THR
1	B	136	SER
1	B	159	VAL
1	B	162	LEU
1	B	169	ARG
1	B	171	VAL
1	B	193	LEU
1	B	244	LEU

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Mol	Chain	Res	Type
1	B	246	VAL
1	B	257	THR
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	360	PRO
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	550	ARG
1	B	555	LEU
1	B	577	LEU
1	B	579	VAL
1	B	587	GLU
1	B	589	THR
1	B	595	LEU
1	B	604	GLN
1	B	605	VAL
1	B	612	ASP
1	B	647	ASN
1	B	648	LYS

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Mol	Chain	Res	Type
1	B	657	VAL
1	B	661	LEU
1	B	666	LEU
1	B	674	LEU
1	B	682	VAL
1	B	684	VAL
1	B	721	LYS
1	B	730	VAL
1	B	737	ASP
1	B	750	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	91	ASN
1	A	119	HIS
1	A	155	ASN
1	A	160	GLN
1	A	164	GLN
1	A	215	GLN
1	A	309	HIS
1	A	364	GLN
1	A	440	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	29	HIS
1	B	80	ASN
1	B	91	ASN
1	B	164	GLN
1	B	196	ASN
1	B	215	GLN
1	B	309	HIS
1	B	440	GLN
1	B	459	GLN
1	B	470	GLN
1	B	507	HIS
1	B	564	ASN

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Mol	Chain	Res	Type
1	B	638	HIS
1	B	647	ASN
1	B	679	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

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%)	-0.17	22 (3%)	50 22	21, 44, 79, 97	0
1	B	723/782 (92%)	-0.13	29 (4%)	38 15	21, 44, 83, 97	0
All	All	1451/1564 (92%)	-0.15	51 (3%)	44 18	21, 44, 81, 97	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	ASP	6.2
1	A	155	ASN	5.0
1	B	375	THR	4.6
1	A	755	ALA	4.6
1	B	531	THR	4.3
1	B	155	ASN	4.1
1	A	156	GLU	3.8
1	A	154	PRO	3.8
1	B	379	GLY	3.8
1	A	372	PRO	3.7
1	B	27	VAL	3.4
1	B	280	ALA	3.4
1	B	373	ASP	3.2
1	B	649	ILE	3.0
1	A	649	ILE	3.0
1	B	532	ALA	2.9
1	B	377	GLY	2.9
1	B	374	GLN	2.8
1	A	532	ALA	2.7
1	A	399	THR	2.7
1	B	378	LEU	2.6
1	A	257	THR	2.6
1	B	257	THR	2.6
1	B	381	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	278	ASN	2.6
1	A	752	GLU	2.5
1	A	375	THR	2.5
1	A	402	THR	2.5
1	B	282	THR	2.5
1	B	228	ARG	2.4
1	A	376	ASP	2.3
1	A	572	PRO	2.3
1	B	255	ALA	2.3
1	A	753	LEU	2.3
1	B	623	ALA	2.3
1	A	530	GLN	2.3
1	A	739	ASP	2.3
1	B	599	ARG	2.3
1	B	754	ALA	2.2
1	A	573	SER	2.2
1	A	280	ALA	2.2
1	B	488	GLU	2.2
1	B	458	ARG	2.2
1	B	530	GLN	2.2
1	B	279	GLY	2.1
1	A	601	GLN	2.1
1	B	372	PRO	2.1
1	B	648	LYS	2.1
1	B	739	ASP	2.1
1	A	620	GLY	2.0
1	A	343	ASP	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

There are no such residues in this entry.