



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:33 am BST

PDB ID : 6JEH  
Title : Crystal structure of calcium free human gelsolin amyloid mutant D187Y  
Authors : Zorgati, H.; Robinson, R.C.  
Deposited on : 2019-02-05  
Resolution : 2.95 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](mailto: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.

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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

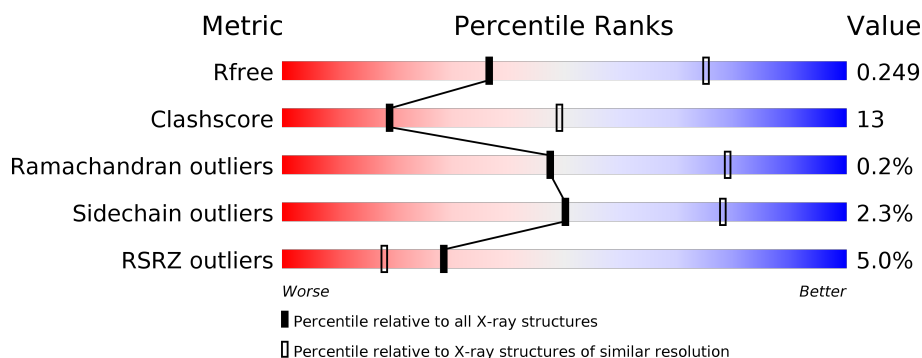
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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  $\geq 3$ , 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	727	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>• •</div> </div> </div>
1	B	727	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11005 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	708	Total	C	N	O	S	0	0	0
			5534	3497	967	1054	16			
1	B	700	Total	C	N	O	S	0	0	0
			5471	3459	956	1040	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	TYR	ASP	engineered mutation	UNP P06396
B	187	TYR	ASP	engineered mutation	UNP P06396

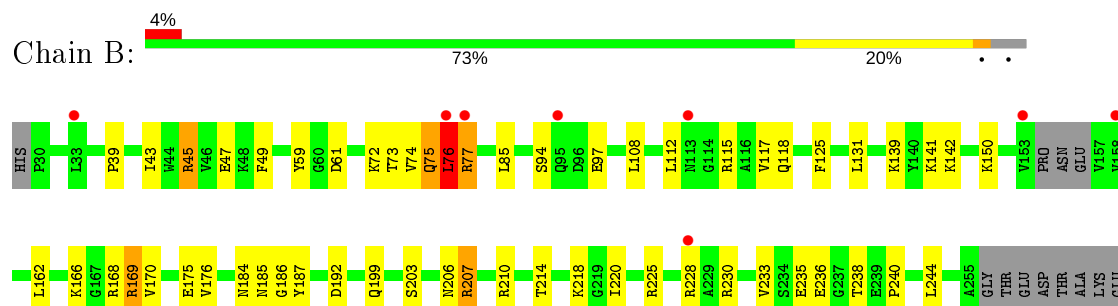
### 3 Residue-property plots

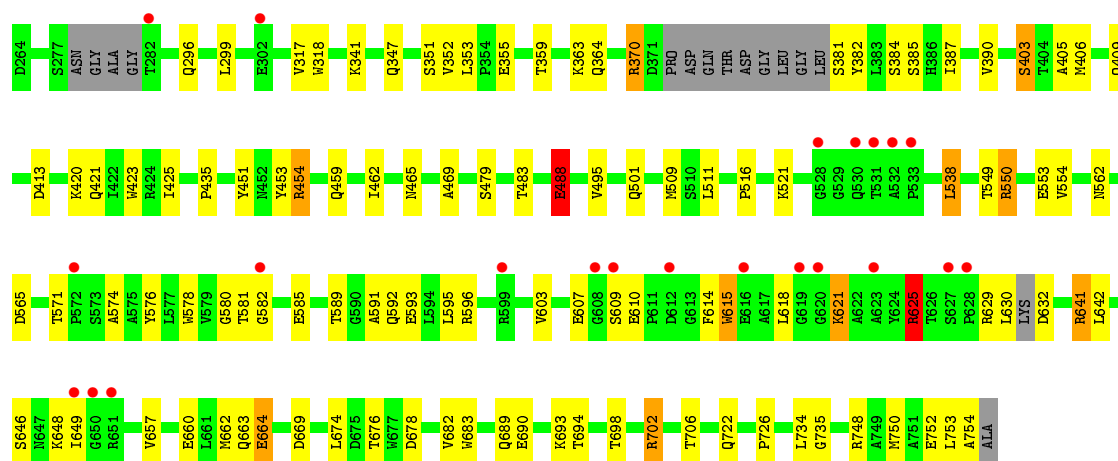
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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



#### • Molecule 1: Gelsolin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.23Å 169.23Å 151.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.95 19.94 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.94-2.95) 98.9 (19.94-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.93Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.193 , 0.249 0.195 , 0.249	Depositor DCC
$R_{free}$ test set	2386 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.54	3/5660 (0.1%)	0.77	8/7664 (0.1%)
1	B	0.57	4/5594 (0.1%)	0.83	12/7571 (0.2%)
All	All	0.56	7/11254 (0.1%)	0.80	20/15235 (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
1	B	0	2
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	585	GLU	CB-CG	10.00	1.71	1.52
1	B	488	GLU	CD-OE2	6.55	1.32	1.25
1	B	230	ARG	CB-CG	-6.07	1.36	1.52
1	A	649	ILE	CB-CG2	6.06	1.71	1.52
1	B	488	GLU	CG-CD	6.01	1.60	1.51
1	A	691	GLU	CB-CG	5.75	1.63	1.52
1	A	93	CYS	CB-SG	-5.59	1.72	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ARG	NE-CZ-NH2	-19.03	110.79	120.30
1	B	230	ARG	NE-CZ-NH1	16.12	128.36	120.30
1	A	555	LEU	CB-CG-CD2	-11.97	90.65	111.00
1	B	664	GLU	CA-CB-CG	-10.08	91.22	113.40
1	A	649	ILE	CG1-CB-CG2	7.79	128.53	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	641	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	378	LEU	CA-CB-CG	7.31	132.10	115.30
1	B	45	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	625	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	B	230	ARG	CG-CD-NE	-6.21	98.76	111.80
1	A	555	LEU	CB-CG-CD1	5.58	120.49	111.00
1	A	588	LYS	CB-CG-CD	-5.43	97.49	111.60
1	B	625	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	538	LEU	CA-CB-CG	5.40	127.72	115.30
1	B	625	ARG	CB-CG-CD	5.40	125.63	111.60
1	A	621	LYS	CB-CA-C	5.35	121.10	110.40
1	A	621	LYS	N-CA-CB	-5.35	100.97	110.60
1	B	207	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	664	GLU	N-CA-CB	-5.18	101.27	110.60
1	B	585	GLU	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	648	LYS	Peptide
1	B	488	GLU	Sidechain
1	B	75	GLN	Mainchain

## 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	5534	0	5390	159	0
1	B	5471	0	5332	129	0
All	All	11005	0	10722	282	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 13.

All (282) 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:370:ARG:NH1	1:A:627:SER:HB3	1.10	1.42
1:A:370:ARG:NH1	1:A:627:SER:CB	1.85	1.39
1:A:648:LYS:O	1:A:649:ILE:HG22	1.37	1.20
1:A:370:ARG:HH11	1:A:627:SER:CB	1.56	1.11
1:B:521:LYS:HG3	1:B:553:GLU:HG2	1.39	1.04
1:A:630:LEU:O	1:A:632:ASP:N	1.92	1.02
1:B:465:ASN:HB2	1:B:483:THR:HG21	1.37	1.01
1:B:75:GLN:O	1:B:76:LEU:O	1.80	0.99
1:A:34:LYS:O	1:A:37:LYS:NZ	1.98	0.96
1:B:630:LEU:O	1:B:632:ASP:N	2.01	0.94
1:A:43:ILE:HG12	1:A:70:ILE:HD12	1.53	0.90
1:A:648:LYS:O	1:A:649:ILE:CG2	2.19	0.90
1:A:185:ASN:ND2	1:A:236:GLU:OE1	2.04	0.89
1:A:713:ARG:H	1:A:713:ARG:HD3	1.38	0.89
1:A:55:PRO:HG2	1:A:58:LEU:HD12	1.56	0.88
1:A:536:THR:HG22	1:A:571:THR:HA	1.54	0.87
1:A:686:LYS:H	1:A:722:GLN:NE2	1.75	0.84
1:A:521:LYS:HG3	1:A:553:GLU:HG2	1.63	0.81
1:B:425:ILE:HD13	1:B:479:SER:HB3	1.65	0.79
1:A:36:GLY:H	1:A:42:GLN:HE22	1.32	0.78
1:A:420:LYS:NZ	1:A:511:LEU:O	2.16	0.77
1:A:379:GLY:H	1:A:633:LYS:HE2	1.50	0.77
1:B:45:ARG:NH1	1:B:47:GLU:OE2	2.17	0.77
1:A:519:ILE:HD12	1:A:552:VAL:HG12	1.66	0.76
1:B:576:TYR:HE2	1:B:614:PHE:HA	1.48	0.76
1:A:370:ARG:HH12	1:A:627:SER:CB	1.74	0.75
1:B:75:GLN:O	1:B:76:LEU:C	2.22	0.74
1:B:571:THR:HG23	1:B:574:ALA:H	1.53	0.74
1:A:625:ARG:NH1	1:A:627:SER:OG	2.20	0.73
1:A:269:LYS:HE2	1:A:705:GLU:O	1.88	0.72
1:A:393:VAL:HA	1:B:459:GLN:NE2	2.05	0.72
1:A:370:ARG:HH12	1:A:627:SER:HB3	0.83	0.72
1:A:70:ILE:HG13	1:A:130:PHE:HE1	1.54	0.72
1:B:185:ASN:ND2	1:B:236:GLU:OE2	2.22	0.71
1:A:371:ASP:OD1	1:A:372:PRO:HD2	1.89	0.71
1:B:296:GLN:HE22	1:B:370:ARG:H	1.38	0.70
1:B:364:GLN:HE22	1:B:641:ARG:NH2	1.89	0.70
1:A:118:GLN:HB2	1:A:352:VAL:HG22	1.74	0.70
1:A:393:VAL:HA	1:B:459:GLN:HE22	1.57	0.70
1:B:576:TYR:CE2	1:B:614:PHE:HA	2.27	0.69
1:B:752:GLU:HG2	1:B:753:LEU:HD22	1.74	0.69
1:B:615:TRP:CD2	1:B:621:LYS:HD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PRO:HA	1:B:73:THR:O	1.93	0.68
1:B:479:SER:O	1:B:483:THR:HG23	1.93	0.68
1:B:214:THR:O	1:B:218:LYS:HG2	1.94	0.68
1:A:91:ASN:H	1:A:123:GLN:NE2	1.92	0.68
1:B:318:TRP:CZ2	1:B:355:GLU:HB2	2.29	0.67
1:A:169:ARG:HD2	1:A:657:VAL:HG12	1.75	0.67
1:A:318:TRP:CZ2	1:A:355:GLU:HB2	2.29	0.67
1:A:139:LYS:HE2	1:A:220:ILE:HG12	1.77	0.67
1:B:207:ARG:HA	1:B:210:ARG:HG3	1.76	0.67
1:B:192:ASP:OD2	1:B:225:ARG:NH2	2.27	0.67
1:A:538:LEU:HG	1:A:556:PRO:HA	1.78	0.66
1:B:185:ASN:OD1	1:B:203:SER:N	2.29	0.66
1:A:571:THR:OG1	1:A:572:PRO:HD2	1.96	0.66
1:A:45:ARG:HH22	1:A:150:LYS:HA	1.61	0.65
1:B:139:LYS:HE2	1:B:220:ILE:HG12	1.79	0.65
1:B:364:GLN:HE22	1:B:641:ARG:HH22	1.43	0.65
1:A:610:GLU:OE1	1:A:610:GLU:N	2.30	0.64
1:A:36:GLY:H	1:A:42:GLN:NE2	1.94	0.63
1:B:199:GLN:HE22	1:B:214:THR:HA	1.63	0.63
1:A:509:MET:HG2	1:A:550:ARG:HD3	1.79	0.63
1:A:169:ARG:NH2	1:A:670:ASP:OD2	2.28	0.63
1:B:184:ASN:OD1	1:B:185:ASN:N	2.33	0.62
1:B:420:LYS:HE2	1:B:511:LEU:HB3	1.81	0.62
1:A:233:VAL:HG11	1:A:750:MET:HE1	1.82	0.62
1:A:143:GLY:HA3	1:A:149:PHE:HD2	1.65	0.62
1:A:323:ALA:O	1:A:328:ARG:NH1	2.32	0.61
1:A:413:ASP:OD2	1:A:726:PRO:HB2	1.99	0.61
1:A:558:ALA:HA	1:A:561:LEU:HD23	1.81	0.61
1:B:413:ASP:OD2	1:B:726:PRO:HB2	2.00	0.61
1:B:206:ASN:OD1	1:B:207:ARG:N	2.35	0.60
1:A:576:TYR:CE2	1:A:614:PHE:HB2	2.36	0.60
1:B:593:GLU:OE1	1:B:596:ARG:NH2	2.35	0.59
1:A:394:PRO:HD3	1:B:459:GLN:NE2	2.18	0.59
1:B:516:PRO:HB3	1:B:549:THR:HB	1.85	0.59
1:B:75:GLN:C	1:B:76:LEU:O	2.41	0.59
1:A:642:LEU:HD23	1:A:657:VAL:HG21	1.84	0.59
1:A:168:ARG:HH12	1:A:208:TYR:HB3	1.68	0.59
1:B:698:THR:O	1:B:702:ARG:HG2	2.02	0.58
1:A:713:ARG:CD	1:A:713:ARG:H	2.15	0.58
1:B:702:ARG:O	1:B:706:THR:HG23	2.02	0.58
1:A:557:LYS:HG3	1:A:559:GLY:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HD11	1:B:108:LEU:HB3	1.85	0.58
1:B:74:VAL:HG21	1:B:385:SER:HB2	1.85	0.58
1:B:425:ILE:HD13	1:B:479:SER:CB	2.32	0.58
1:A:370:ARG:HH11	1:A:627:SER:HB2	1.63	0.57
1:B:43:ILE:HD12	1:B:59:TYR:CG	2.40	0.57
1:A:504:GLU:OE1	1:A:550:ARG:NH1	2.38	0.56
1:A:584:SER:OG	1:A:587:GLU:OE2	2.20	0.56
1:B:683:TRP:CZ2	1:B:722:GLN:HB2	2.40	0.56
1:A:434:ASP:HB3	1:A:437:THR:HG22	1.87	0.56
1:B:61:ASP:HB3	1:B:141:LYS:HD2	1.87	0.56
1:B:615:TRP:CD1	1:B:618:LEU:HD12	2.40	0.56
1:A:85:LEU:HD11	1:A:108:LEU:HB3	1.88	0.56
1:B:168:ARG:NH2	1:B:669:ASP:OD1	2.39	0.56
1:A:557:LYS:HE3	1:A:558:ALA:H	1.70	0.56
1:A:664:GLU:OE1	1:A:664:GLU:N	2.31	0.56
1:A:734:LEU:HD12	1:A:735:GLY:N	2.21	0.56
1:B:184:ASN:OD1	1:B:186:GLY:N	2.27	0.55
1:A:70:ILE:HG13	1:A:130:PHE:CE1	2.40	0.55
1:B:592:GLN:HA	1:B:595:LEU:HD23	1.89	0.55
1:A:43:ILE:HD12	1:A:59:TYR:CG	2.43	0.54
1:A:237:GLY:N	1:A:239:GLU:OE2	2.40	0.54
1:A:57:ASN:HD21	1:A:153:VAL:HG11	1.73	0.54
1:A:370:ARG:NH1	1:A:627:SER:OG	2.36	0.53
1:B:405:ALA:O	1:B:409:GLN:HG3	2.08	0.53
1:A:425:ILE:HG13	1:A:479:SER:HB3	1.91	0.53
1:B:591:ALA:O	1:B:595:LEU:CD2	2.56	0.53
1:A:183:PHE:HA	1:A:189:PHE:CZ	2.43	0.53
1:A:557:LYS:HG3	1:A:558:ALA:N	2.23	0.53
1:A:422:ILE:HG12	1:A:449:ILE:CG1	2.39	0.53
1:B:509:MET:HG2	1:B:550:ARG:HB3	1.90	0.53
1:A:690:GLU:O	1:A:694:THR:HG23	2.09	0.53
1:A:595:LEU:HD13	1:A:602:PRO:HB3	1.91	0.53
1:B:538:LEU:HB3	1:B:554:VAL:HG23	1.90	0.52
1:A:218:LYS:NZ	1:A:222:ASP:OD2	2.40	0.52
1:A:394:PRO:HD3	1:B:459:GLN:HE21	1.74	0.52
1:A:235:GLU:HG2	1:A:236:GLU:H	1.73	0.52
1:A:516:PRO:HB3	1:A:549:THR:OG1	2.07	0.52
1:A:509:MET:CE	1:A:550:ARG:HE	2.23	0.52
1:B:465:ASN:CB	1:B:483:THR:HG21	2.24	0.52
1:B:454:ARG:HG2	1:B:454:ARG:HH11	1.75	0.51
1:B:387:ILE:HG13	1:B:387:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG21	1:A:212:LYS:HB3	1.93	0.51
1:B:662:MET:HB3	1:B:664:GLU:OE1	2.10	0.51
1:B:317:VAL:HB	1:B:352:VAL:HG12	1.93	0.51
1:A:702:ARG:O	1:A:706:THR:HG23	2.10	0.51
1:B:118:GLN:HB2	1:B:352:VAL:HG22	1.93	0.51
1:A:400:LEU:CD2	1:A:414:ASP:HA	2.41	0.51
1:B:646:SER:OG	1:B:648:LYS:HG2	2.11	0.51
1:A:686:LYS:H	1:A:722:GLN:HE21	1.55	0.51
1:A:394:PRO:CD	1:B:459:GLN:HE21	2.23	0.51
1:A:405:ALA:O	1:A:409:GLN:HG3	2.11	0.51
1:A:576:TYR:HD1	1:A:603:VAL:HG22	1.76	0.50
1:B:142:LYS:HE3	1:B:175:GLU:HG2	1.93	0.50
1:B:469:ALA:H	1:B:501:GLN:HE21	1.59	0.50
1:B:581:THR:HG23	1:B:607:GLU:OE2	2.11	0.50
1:B:615:TRP:CE3	1:B:621:LYS:HD2	2.46	0.50
1:A:336:SER:O	1:A:340:THR:HG23	2.12	0.50
1:A:519:ILE:CD1	1:A:552:VAL:HG12	2.40	0.50
1:A:422:ILE:HG12	1:A:449:ILE:HG13	1.93	0.49
1:B:168:ARG:HH12	1:B:206:ASN:ND2	2.10	0.49
1:B:387:ILE:HD12	1:B:390:VAL:HG21	1.94	0.49
1:B:591:ALA:O	1:B:595:LEU:HD23	2.13	0.49
1:B:117:VAL:HG13	1:B:353:LEU:HD23	1.93	0.49
1:A:563:SER:OG	1:A:626:THR:HG22	2.12	0.49
1:A:610:GLU:HG2	1:A:611:PRO:O	2.12	0.49
1:A:135:LYS:HE2	1:A:662:MET:HE2	1.93	0.49
1:B:39:PRO:HA	1:B:73:THR:HG22	1.94	0.49
1:A:576:TYR:CD2	1:A:614:PHE:HD1	2.31	0.49
1:A:91:ASN:H	1:A:123:GLN:HE21	1.59	0.49
1:A:648:LYS:HG2	1:A:649:ILE:H	1.78	0.48
1:B:403:SER:OG	1:B:406:MET:HB3	2.14	0.48
1:B:565:ASP:OD2	1:B:629:ARG:NH2	2.43	0.48
1:A:37:LYS:H	1:A:37:LYS:HD3	1.79	0.48
1:A:465:ASN:HD21	1:A:467:GLN:HE21	1.61	0.48
1:A:562:ASN:ND2	1:A:629:ARG:HH22	2.11	0.48
1:B:609:SER:N	1:B:610:GLU:OE1	2.47	0.48
1:A:43:ILE:HG23	1:A:70:ILE:CD1	2.44	0.48
1:B:689:GLN:O	1:B:693:LYS:HG3	2.14	0.48
1:A:713:ARG:HG2	1:A:714:ARG:HG3	1.96	0.48
1:A:683:TRP:CZ2	1:A:722:GLN:HB2	2.49	0.48
1:B:734:LEU:HD12	1:B:735:GLY:H	1.79	0.48
1:B:94:SER:HB3	1:B:97:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:H	1:A:238:THR:CG2	2.27	0.47
1:A:465:ASN:ND2	1:A:467:GLN:HE21	2.12	0.47
1:B:168:ARG:HH11	1:B:168:ARG:HG3	1.79	0.47
1:B:642:LEU:O	1:B:657:VAL:HG13	2.14	0.47
1:A:373:ASP:O	1:A:375:THR:N	2.46	0.47
1:A:36:GLY:N	1:A:42:GLN:HE22	2.08	0.47
1:B:77:ARG:CG	1:B:77:ARG:HH21	2.27	0.47
1:A:76:LEU:O	1:A:78:ASN:N	2.42	0.47
1:A:534:ALA:HB3	1:A:537:ARG:HG2	1.96	0.47
1:A:135:LYS:HE2	1:A:662:MET:CE	2.44	0.47
1:A:139:LYS:HG2	1:A:173:ALA:HB3	1.95	0.47
1:A:498:ARG:NH1	1:A:500:VAL:HG13	2.30	0.47
1:B:61:ASP:OD1	1:B:139:LYS:NZ	2.39	0.47
1:A:558:ALA:N	1:A:618:LEU:HD12	2.30	0.47
1:B:77:ARG:HG3	1:B:77:ARG:NH2	2.29	0.47
1:B:233:VAL:HG11	1:B:750:MET:SD	2.55	0.47
1:A:576:TYR:HE2	1:A:614:PHE:HA	1.80	0.47
1:A:95:GLN:H	1:A:95:GLN:CD	2.18	0.47
1:B:125:PHE:CE1	1:B:347:GLN:HG2	2.50	0.47
1:A:400:LEU:HD22	1:A:414:ASP:HA	1.97	0.46
1:B:421:GLN:HG2	1:B:423:TRP:CZ2	2.50	0.46
1:A:360:PRO:O	1:A:364:GLN:HG3	2.15	0.46
1:B:225:ARG:O	1:B:228:ARG:HB2	2.14	0.46
1:B:77:ARG:O	1:B:77:ARG:HG3	2.15	0.46
1:A:168:ARG:NH2	1:A:669:ASP:OD1	2.48	0.46
1:B:169:ARG:HG2	1:B:169:ARG:H	1.43	0.46
1:A:580:GLY:HA2	1:A:607:GLU:HB2	1.97	0.46
1:A:206:ASN:ND2	1:A:209:GLU:HG3	2.30	0.46
1:B:131:LEU:HD13	1:B:170:VAL:CG1	2.45	0.46
1:B:210:ARG:O	1:B:214:THR:HG23	2.16	0.46
1:A:221:ARG:HH12	1:A:753:LEU:HB3	1.80	0.46
1:A:558:ALA:HA	1:A:561:LEU:CD2	2.45	0.46
1:B:384:SER:O	1:B:387:ILE:HG22	2.16	0.46
1:B:359:THR:O	1:B:363:LYS:HG3	2.16	0.46
1:B:562:ASN:HA	1:B:625:ARG:O	2.16	0.46
1:A:287:LEU:HD21	1:A:290:ASP:HB3	1.98	0.46
1:A:689:GLN:O	1:A:693:LYS:HG3	2.16	0.46
1:A:576:TYR:HD2	1:A:614:PHE:HD1	1.63	0.46
1:B:748:ARG:O	1:B:752:GLU:N	2.33	0.46
1:A:230:ARG:HG2	1:A:232:HIS:CE1	2.51	0.45
1:B:462:ILE:HG23	1:B:495:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASP:OD2	1:A:496:GLN:NE2	2.49	0.45
1:A:615:TRP:HD1	1:A:615:TRP:HA	1.57	0.45
1:A:740:TYR:O	1:A:748:ARG:NH2	2.45	0.45
1:B:240:PRO:O	1:B:244:LEU:HD12	2.17	0.45
1:A:538:LEU:CD1	1:A:554:VAL:HG13	2.48	0.44
1:A:575:ALA:HB3	1:A:601:GLN:O	2.17	0.44
1:B:118:GLN:O	1:B:351:SER:HA	2.17	0.44
1:B:207:ARG:HG2	1:B:210:ARG:NH1	2.32	0.44
1:A:336:SER:OG	1:A:346:LYS:NZ	2.31	0.44
1:A:57:ASN:HD21	1:A:153:VAL:CG1	2.30	0.44
1:A:734:LEU:HD12	1:A:735:GLY:H	1.81	0.44
1:B:72:LYS:HE3	1:B:74:VAL:HG23	1.99	0.44
1:A:66:ASP:OD1	1:A:145:VAL:HG12	2.17	0.44
1:A:346:LYS:HA	1:A:346:LYS:HD2	1.85	0.44
1:A:339:ILE:HG23	1:A:344:TYR:HB2	1.98	0.44
1:A:37:LYS:HD3	1:A:37:LYS:N	2.31	0.44
1:A:360:PRO:HB3	1:A:637:ALA:O	2.18	0.44
1:B:43:ILE:HD12	1:B:59:TYR:CD2	2.53	0.44
1:B:454:ARG:HG2	1:B:454:ARG:NH1	2.32	0.44
1:A:648:LYS:C	1:A:649:ILE:HG22	2.29	0.44
1:A:685:GLY:HA2	1:A:722:GLN:HE21	1.83	0.44
1:B:112:LEU:O	1:B:115:ARG:HG2	2.17	0.44
1:B:690:GLU:O	1:B:694:THR:HG23	2.18	0.44
1:B:299:LEU:HD13	1:B:318:TRP:CE2	2.53	0.44
1:A:569:LEU:HD22	1:A:618:LEU:HD21	1.99	0.43
1:B:451:TYR:CE1	1:B:511:LEU:HD22	2.53	0.43
1:B:648:LYS:O	1:B:649:ILE:HG22	2.19	0.43
1:A:43:ILE:HD12	1:A:59:TYR:CD2	2.53	0.43
1:A:178:VAL:HG23	1:A:178:VAL:O	2.18	0.43
1:B:299:LEU:HD13	1:B:318:TRP:CD2	2.54	0.43
1:B:580:GLY:HA2	1:B:607:GLU:HB2	2.00	0.43
1:A:603:VAL:HG23	1:A:603:VAL:O	2.19	0.43
1:B:663:GLN:N	1:B:664:GLU:OE1	2.52	0.43
1:A:184:ASN:H	1:A:189:PHE:HZ	1.66	0.43
1:A:370:ARG:NH1	1:A:627:SER:HB2	2.13	0.43
1:A:376:ASP:HB2	1:B:435:PRO:HB3	2.00	0.43
1:A:592:GLN:HA	1:A:595:LEU:HD12	2.00	0.43
1:B:750:MET:O	1:B:754:ALA:HB3	2.18	0.42
1:A:571:THR:HG22	1:A:574:ALA:O	2.20	0.42
1:B:660:GLU:O	1:B:662:MET:HG3	2.19	0.42
1:B:603:VAL:HG23	1:B:603:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ALA:O	1:A:658:PRO:HB3	2.19	0.42
1:A:640:PRO:HA	1:A:675:ASP:O	2.19	0.42
1:B:166:LYS:HD3	1:B:187:TYR:CE2	2.54	0.42
1:B:578:TRP:HZ2	1:B:607:GLU:HG3	1.84	0.42
1:A:269:LYS:O	1:A:269:LYS:HG3	2.20	0.42
1:A:555:LEU:HA	1:A:556:PRO:HD3	1.74	0.42
1:A:269:LYS:HE3	1:A:269:LYS:HB2	1.78	0.42
1:A:746:LEU:HD11	1:A:750:MET:HE3	2.00	0.42
1:A:674:LEU:HB3	1:A:681:PHE:HB2	2.02	0.42
1:B:168:ARG:NH1	1:B:206:ASN:ND2	2.68	0.42
1:A:359:THR:O	1:A:363:LYS:HG3	2.19	0.41
1:A:614:PHE:CE2	1:A:615:TRP:NE1	2.88	0.41
1:B:235:GLU:H	1:B:238:THR:CG2	2.32	0.41
1:B:538:LEU:HA	1:B:538:LEU:HD23	1.85	0.41
1:B:589:THR:HA	1:B:592:GLN:HE21	1.85	0.41
1:A:200:TRP:HA	1:A:234:SER:O	2.21	0.41
1:A:135:LYS:NZ	1:A:658:PRO:O	2.45	0.41
1:A:292:ASN:HB2	1:A:293:PRO:HA	2.02	0.41
1:A:660:GLU:O	1:A:662:MET:HG3	2.20	0.41
1:B:676:THR:HG22	1:B:678:ASP:H	1.85	0.41
1:B:76:LEU:HD12	1:B:76:LEU:HA	1.74	0.41
1:A:95:GLN:N	1:A:95:GLN:OE1	2.54	0.40
1:B:45:ARG:HH22	1:B:150:LYS:HD3	1.86	0.40
1:B:381:SER:OG	1:B:382:TYR:N	2.53	0.40
1:B:451:TYR:HE2	1:B:453:TYR:HB3	1.86	0.40
1:A:233:VAL:HG11	1:A:750:MET:CE	2.51	0.40
1:B:170:VAL:O	1:B:170:VAL:HG23	2.22	0.40
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.82	0.40
1:A:29:HIS:O	1:A:32:PHE:HB2	2.21	0.40
1:B:77:ARG:CG	1:B:77:ARG:NH2	2.83	0.40
1:A:185:ASN:OD1	1:A:203:SER:N	2.54	0.40
1:B:162:LEU:HD23	1:B:176:VAL:HG23	2.02	0.40
1:B:581:THR:OG1	1:B:582:GLY:N	2.55	0.40
1:B:625:ARG:NE	1:B:625:ARG:HA	2.37	0.40
1:B:97:GLU:HA	1:B:97:GLU:OE2	2.22	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	698/727 (96%)	677 (97%)	19 (3%)	2 (0%)	41	73
1	B	688/727 (95%)	667 (97%)	20 (3%)	1 (0%)	51	83
All	All	1386/1454 (95%)	1344 (97%)	39 (3%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	GLN
1	B	76	LEU
1	A	649	ILE

### 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	579/591 (98%)	570 (98%)	9 (2%)	62	84
1	B	571/591 (97%)	554 (97%)	17 (3%)	41	72
All	All	1150/1182 (97%)	1124 (98%)	26 (2%)	50	78

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	45	ARG
1	A	49	PHE

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Mol	Chain	Res	Type
1	A	384	SER
1	A	538	LEU
1	A	557	LYS
1	A	596	ARG
1	A	713	ARG
1	A	721	LYS
1	B	49	PHE
1	B	76	LEU
1	B	77	ARG
1	B	169	ARG
1	B	341	LYS
1	B	370	ARG
1	B	403	SER
1	B	454	ARG
1	B	488	GLU
1	B	538	LEU
1	B	550	ARG
1	B	615	TRP
1	B	621	LYS
1	B	625	ARG
1	B	674	LEU
1	B	682	VAL
1	B	702	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	42	GLN
1	A	123	GLN
1	A	223	ASN
1	A	245	GLN
1	A	465	ASN
1	A	496	GLN
1	A	722	GLN
1	B	42	GLN
1	B	199	GLN
1	B	296	GLN
1	B	364	GLN
1	B	401	HIS
1	B	459	GLN
1	B	470	GLN
1	B	501	GLN

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Mol	Chain	Res	Type
1	B	592	GLN
1	B	663	GLN
1	B	710	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	708/727 (97%)	0.06	40 (5%) 24 15	30, 60, 127, 167	0
1	B	700/727 (96%)	-0.06	30 (4%) 35 22	26, 56, 107, 143	0
All	All	1408/1454 (96%)	-0.00	70 (4%) 28 18	26, 58, 117, 167	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	649	ILE	6.1
1	B	530	GLN	5.2
1	A	532	ALA	4.7
1	A	649	ILE	4.6
1	A	576	TYR	4.2
1	A	531	THR	4.1
1	A	255	ALA	4.1
1	A	597	VAL	3.9
1	B	282	THR	3.8
1	A	599	ARG	3.7
1	B	650	GLY	3.6
1	A	573	SER	3.6
1	A	529	GLY	3.5
1	A	616	GLU	3.5
1	A	620	GLY	3.5
1	A	622	ALA	3.5
1	A	609	SER	3.4
1	B	77	ARG	3.3
1	A	623	ALA	3.2
1	B	532	ALA	3.0
1	B	531	THR	3.0
1	A	568	VAL	3.0
1	A	533	PRO	3.0
1	A	528	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	650	GLY	3.0
1	B	528	GLY	2.9
1	B	582	GLY	2.9
1	A	648	LYS	2.9
1	B	651	ARG	2.8
1	B	609	SER	2.7
1	B	620	GLY	2.7
1	B	33	LEU	2.7
1	B	228	ARG	2.7
1	A	608	GLY	2.7
1	A	539	PHE	2.6
1	A	601	GLN	2.6
1	B	599	ARG	2.6
1	A	282	THR	2.6
1	A	228	ARG	2.5
1	B	619	GLY	2.5
1	B	628	PRO	2.5
1	B	158	VAL	2.5
1	A	651	ARG	2.5
1	B	113	ASN	2.5
1	A	95	GLN	2.5
1	A	600	ALA	2.4
1	A	626	THR	2.4
1	B	533	PRO	2.4
1	B	616	GLU	2.4
1	B	608	GLY	2.4
1	A	613	GLY	2.4
1	A	530	GLN	2.3
1	A	611	PRO	2.3
1	A	582	GLY	2.3
1	B	95	GLN	2.3
1	A	153	VAL	2.3
1	A	457	GLY	2.3
1	B	153	VAL	2.3
1	B	612	ASP	2.1
1	B	623	ALA	2.1
1	A	538	LEU	2.1
1	B	302	GLU	2.1
1	A	621	LYS	2.1
1	A	572	PRO	2.1
1	B	627	SER	2.1
1	B	572	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	76	LEU	2.0
1	A	602	PRO	2.0
1	A	195	ASN	2.0
1	A	574	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.