



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2022 – 04:08 pm BST

PDB ID : 5LG5
Title : Crystal structure of allantoin racemase from *Pseudomonas fluorescens* AllR
Authors : Cendron, I.; Zanotti, G.; Percudani, R.; Ragazzina, I.; Puggioni, V.; Maccacaro, E.; Liuzzi, A.; Secchi, A.
Deposited on : 2016-07-06
Resolution : 2.10 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

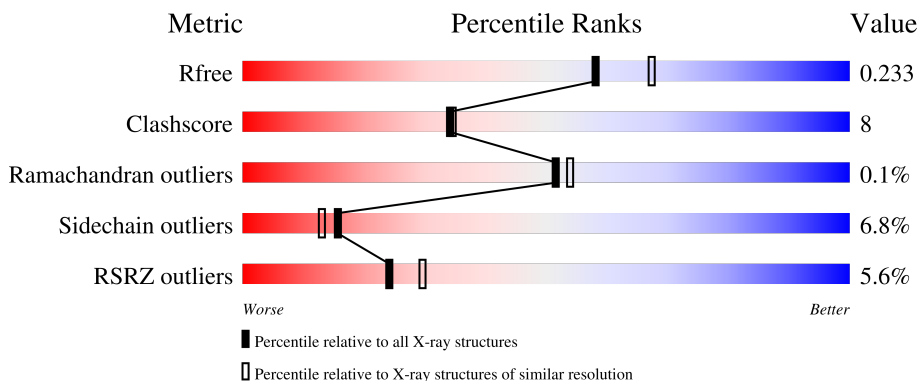
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



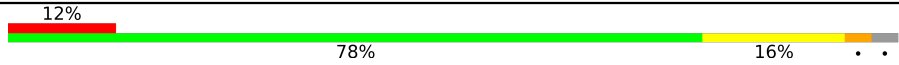
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	242	
1	B	242	
1	C	242	
1	D	242	
1	F	242	

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Mol	Chain	Length	Quality of chain
1	G	242	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '12%', a large green segment in the middle labeled '78%', and a yellow segment on the right labeled '16%'. At the far right end of the bar, there are two small grey dots.</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11434 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 Allantoin racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	236	1763	1107	303	343	10	0	0	0
1	B	235	1749	1096	301	342	10	0	0	0
1	C	236	1763	1107	303	343	10	0	0	0
1	D	236	1763	1107	303	343	10	0	0	0
1	F	237	1770	1112	304	344	10	0	0	0
1	G	235	1749	1096	301	342	10	0	0	0

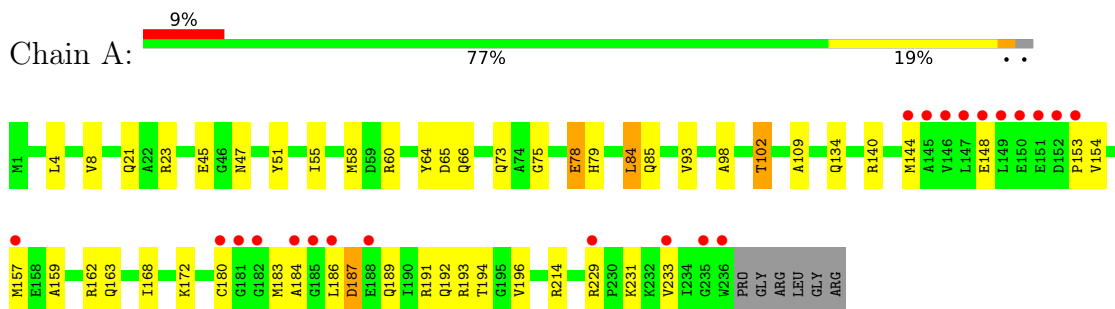
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total 126	O 126	0	0
2	B	135	Total 135	O 135	0	0
2	C	165	Total 165	O 165	0	0
2	D	179	Total 179	O 179	0	0
2	F	139	Total 139	O 139	0	0
2	G	133	Total 133	O 133	0	0

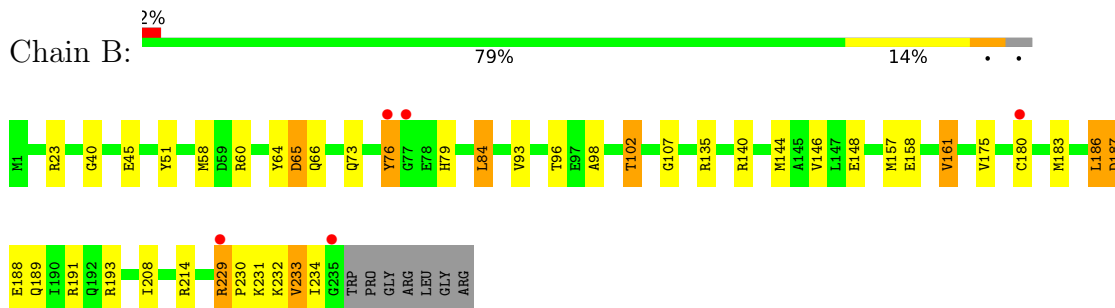
3 Residue-property plots i

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.

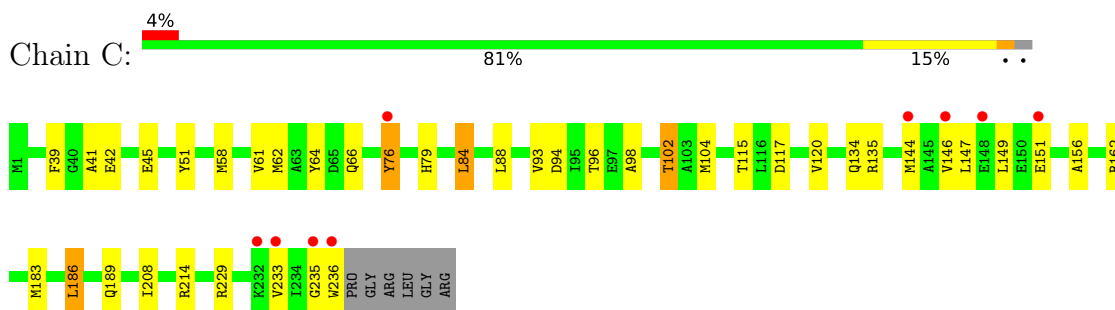
- Molecule 1: Allantoin racemase



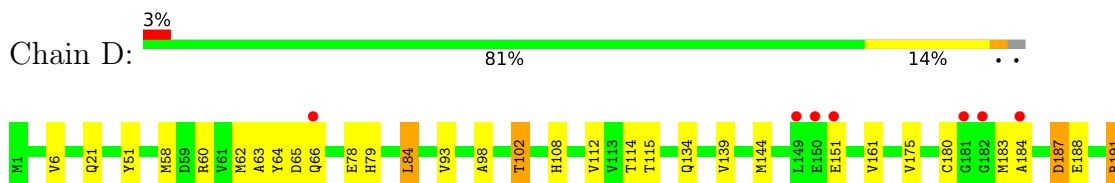
- Molecule 1: Allantoin racemase

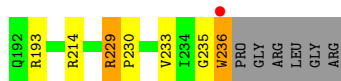


- Molecule 1: Allantoin racemase

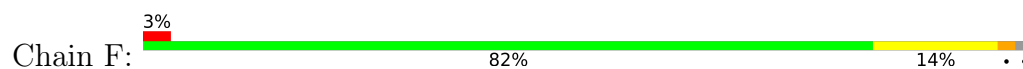


- Molecule 1: Allantoin racemase

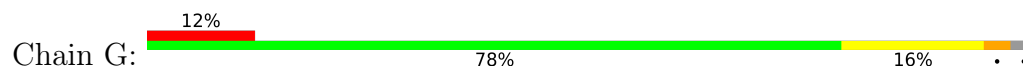




- Molecule 1: Allantoin racemase



- Molecule 1: Allantoin racemase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.22Å 142.32Å 146.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 2.10 39.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.78-2.10) 99.4 (39.78-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.186 , 0.233 0.191 , 0.233	Depositor DCC
R_{free} test set	3720 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.012 for -h,l,k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11434	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/1786	0.60	0/2429
1	B	0.41	0/1770	0.59	0/2406
1	C	0.41	0/1786	0.59	0/2429
1	D	0.43	0/1786	0.66	2/2429 (0.1%)
1	F	0.41	0/1794	0.61	0/2441
1	G	0.41	0/1770	0.61	0/2406
All	All	0.41	0/10692	0.61	2/14540 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	151	GLU	CB-CA-C	-6.09	98.22	110.40
1	D	151	GLU	CA-CB-CG	5.47	125.44	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1793	45	0
1	B	1749	0	1783	37	0
1	C	1763	0	1793	30	0
1	D	1763	0	1793	25	0
1	F	1770	0	1800	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1749	0	1783	35	0
2	A	126	0	0	19	0
2	B	135	0	0	8	1
2	C	165	0	0	8	0
2	D	179	0	0	10	0
2	F	139	0	0	7	2
2	G	133	0	0	10	1
All	All	11434	0	10745	178	2

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 (178) 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:157:MET:SD	2:A:418:HOH:O	2.04	1.13
1:B:140:ARG:NH2	2:B:301:HOH:O	2.00	0.95
1:A:191:ARG:NH1	2:A:302:HOH:O	1.99	0.94
1:A:192:GLN:OE1	2:A:301:HOH:O	1.85	0.93
1:G:28:PRO:O	2:G:301:HOH:O	1.87	0.91
1:D:191:ARG:NH2	2:D:302:HOH:O	2.06	0.89
1:D:64:TYR:O	2:D:301:HOH:O	1.92	0.88
1:D:66:GLN:OE1	2:D:301:HOH:O	1.94	0.85
1:A:140:ARG:NH2	2:A:305:HOH:O	2.09	0.85
1:A:193:ARG:NE	2:A:306:HOH:O	2.11	0.84
1:A:180:CYS:HB3	1:A:183:MET:HG3	1.62	0.81
1:F:158:GLU:OE1	1:F:193:ARG:NH2	2.15	0.79
1:B:45:GLU:OE2	2:B:302:HOH:O	2.00	0.78
1:C:135:ARG:HD2	2:D:453:HOH:O	1.85	0.77
1:G:75:GLY:O	2:G:302:HOH:O	2.01	0.77
1:A:55:ILE:HD11	1:G:52:LEU:HA	1.67	0.76
1:F:76:TYR:O	2:F:302:HOH:O	2.03	0.76
1:G:152:ASP:OD1	2:G:303:HOH:O	2.03	0.76
1:A:73:GLN:NE2	1:A:78:GLU:OE2	2.17	0.75
1:D:98:ALA:O	1:D:102:THR:HG23	1.88	0.73
1:A:23:ARG:O	2:A:304:HOH:O	2.05	0.73
1:C:98:ALA:O	1:C:102:THR:HG23	1.89	0.73
1:A:98:ALA:O	1:A:102:THR:HG23	1.89	0.72
1:F:189:GLN:NE2	2:F:303:HOH:O	2.10	0.72
1:B:229:ARG:NH2	1:B:230:PRO:O	2.24	0.70
1:D:78:GLU:HB2	2:D:316:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:LEU:O	2:G:304:HOH:O	2.10	0.69
1:G:98:ALA:O	1:G:102:THR:HG23	1.93	0.69
1:C:79:HIS:HE1	2:C:308:HOH:O	1.75	0.69
1:A:134:GLN:OE1	2:A:308:HOH:O	2.12	0.68
1:F:162:ARG:NH1	2:F:306:HOH:O	2.22	0.67
2:A:345:HOH:O	1:B:214:ARG:HD2	1.96	0.66
1:B:79:HIS:O	2:B:303:HOH:O	2.13	0.66
1:F:98:ALA:O	1:F:102:THR:HG23	1.95	0.66
1:F:165:GLU:OE1	2:F:304:HOH:O	2.13	0.66
1:D:65:ASP:OD2	2:D:303:HOH:O	2.14	0.66
1:C:94:ASP:OD2	2:C:301:HOH:O	2.13	0.65
1:B:158:GLU:OE2	1:B:193:ARG:NH1	2.26	0.65
1:B:65:ASP:OD1	1:B:65:ASP:N	2.26	0.65
1:D:180:CYS:HB3	1:D:183:MET:HG3	1.78	0.64
1:B:98:ALA:O	1:B:102:THR:HG23	1.98	0.64
1:C:214:ARG:HD2	2:D:390:HOH:O	1.98	0.64
1:D:193:ARG:HD2	2:D:353:HOH:O	1.97	0.63
1:G:104:MET:O	1:G:135:ARG:NH2	2.26	0.63
1:C:62:MET:HG3	1:C:236:TRP:CZ2	2.34	0.62
1:B:234:ILE:HG13	1:C:39:PHE:HA	1.82	0.62
1:G:112:VAL:HG13	1:G:139:VAL:HG22	1.82	0.61
1:C:235:GLY:HA3	2:C:304:HOH:O	2.00	0.61
1:A:58:MET:HG2	1:A:84:LEU:HD13	1.83	0.61
1:C:76:TYR:CE1	1:C:96:THR:HA	2.37	0.59
1:D:112:VAL:HG22	1:D:139:VAL:HG13	1.84	0.59
1:C:79:HIS:CE1	2:C:308:HOH:O	2.52	0.59
1:A:231:LYS:NZ	1:G:45:GLU:OE1	2.32	0.59
1:D:187:ASP:OD1	1:D:187:ASP:N	2.33	0.59
1:G:76:TYR:CE2	1:G:96:THR:HG23	2.37	0.59
1:C:236:TRP:N	2:C:304:HOH:O	2.28	0.59
1:D:58:MET:HG2	1:D:84:LEU:HD13	1.85	0.58
1:G:187:ASP:OD2	1:G:187:ASP:N	2.34	0.58
1:C:64:TYR:CE2	1:C:66:GLN:HB2	2.39	0.58
1:C:58:MET:HG2	1:C:84:LEU:HD13	1.86	0.58
1:G:76:TYR:CE1	1:G:96:THR:HA	2.39	0.58
1:A:64:TYR:CE2	1:A:66:GLN:HB2	2.39	0.57
1:B:58:MET:HG2	1:B:84:LEU:HD13	1.86	0.57
1:B:107:GLY:O	1:B:135:ARG:NH2	2.37	0.57
1:A:172:LYS:NZ	2:A:303:HOH:O	2.04	0.56
1:F:58:MET:HG2	1:F:84:LEU:HD13	1.88	0.56
1:A:162:ARG:HH21	1:A:163:GLN:HE21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ASP:O	1:C:120:VAL:HG13	2.06	0.55
1:D:236:TRP:HA	1:F:39:PHE:CD2	2.41	0.55
1:A:51:TYR:CE1	1:G:79:HIS:HB3	2.42	0.54
1:A:162:ARG:NH2	1:A:163:GLN:HE21	2.05	0.54
1:F:189:GLN:HG2	2:F:303:HOH:O	2.06	0.54
1:B:187:ASP:OD1	1:B:187:ASP:N	2.39	0.54
1:G:188:GLU:N	1:G:188:GLU:OE2	2.36	0.54
1:G:78:GLU:HB2	2:G:330:HOH:O	2.07	0.54
1:D:51:TYR:CE1	1:F:79:HIS:HB3	2.43	0.54
1:G:158:GLU:OE2	1:G:193:ARG:NH2	2.41	0.53
1:A:193:ARG:O	2:A:309:HOH:O	2.18	0.53
1:F:107:GLY:O	1:F:135:ARG:NH2	2.41	0.52
1:F:76:TYR:CE1	1:F:96:THR:HA	2.44	0.52
1:C:62:MET:HG3	1:C:236:TRP:HZ2	1.75	0.52
1:A:187:ASP:OD1	1:A:187:ASP:N	2.43	0.52
1:B:76:TYR:CE2	1:B:96:THR:HG23	2.43	0.52
1:A:55:ILE:CD1	1:G:52:LEU:HA	2.39	0.51
1:A:153:PRO:O	1:A:157:MET:N	2.40	0.51
1:B:64:TYR:CE2	1:B:66:GLN:HB2	2.46	0.51
1:A:157:MET:SD	1:A:186:LEU:HD11	2.50	0.51
1:A:159:ALA:HA	1:A:162:ARG:HH12	1.76	0.51
1:B:76:TYR:CE1	1:B:96:THR:HA	2.46	0.51
1:G:157:MET:O	1:G:161:VAL:HG13	2.10	0.51
1:A:168:ILE:CD1	1:A:194:THR:HB	2.41	0.50
1:D:79:HIS:HB3	1:F:51:TYR:CE1	2.47	0.50
1:A:79:HIS:HE1	2:A:310:HOH:O	1.94	0.50
1:A:65:ASP:N	1:A:65:ASP:OD1	2.44	0.49
1:G:180:CYS:HB3	1:G:183:MET:HG3	1.94	0.49
1:G:8:VAL:HG13	1:G:44:VAL:HG21	1.94	0.49
1:A:214:ARG:NH2	2:A:317:HOH:O	2.46	0.49
1:B:146:VAL:HG23	2:B:302:HOH:O	2.12	0.49
2:A:313:HOH:O	1:B:214:ARG:NH2	2.44	0.49
1:B:188:GLU:HG3	1:B:191:ARG:HH12	1.78	0.49
1:A:109:ALA:HB2	2:A:381:HOH:O	2.12	0.49
1:A:51:TYR:C	1:G:55:ILE:HD11	2.33	0.48
1:F:2:ARG:HD2	1:F:67:PRO:O	2.13	0.48
1:F:214:ARG:HD2	2:G:392:HOH:O	2.13	0.48
1:G:140:ARG:NH2	2:G:311:HOH:O	2.46	0.48
1:A:159:ALA:HA	1:A:162:ARG:NH1	2.27	0.48
1:D:62:MET:O	1:D:63:ALA:HB3	2.13	0.48
1:A:47:ASN:ND2	2:A:310:HOH:O	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ASP:CG	2:G:303:HOH:O	2.48	0.48
1:C:104:MET:O	1:C:135:ARG:NH2	2.47	0.48
1:G:122:LEU:HD23	2:G:348:HOH:O	2.11	0.48
1:F:157:MET:CE	1:F:186:LEU:HG	2.44	0.48
1:D:63:ALA:HA	2:D:350:HOH:O	2.14	0.47
1:G:44:VAL:HG11	1:G:78:GLU:HG2	1.97	0.47
2:B:316:HOH:O	1:D:108:HIS:HE1	1.96	0.47
1:B:40:GLY:HA3	2:B:392:HOH:O	2.14	0.47
1:B:188:GLU:HG3	1:B:191:ARG:NH1	2.29	0.47
1:F:183:MET:O	1:F:186:LEU:HB2	2.14	0.47
1:A:8:VAL:HG11	1:A:78:GLU:HG2	1.96	0.47
1:B:51:TYR:CE1	1:C:79:HIS:HB3	2.50	0.47
1:D:161:VAL:HG21	1:D:193:ARG:HD3	1.97	0.46
1:C:115:THR:HG21	1:C:146:VAL:HG22	1.98	0.46
1:A:45:GLU:OE1	1:G:229:ARG:NE	2.40	0.46
1:F:187:ASP:OD1	1:F:187:ASP:N	2.44	0.45
1:A:180:CYS:O	1:A:183:MET:HB2	2.17	0.45
1:F:72:ILE:HD11	1:F:206:VAL:HA	1.97	0.45
1:A:154:VAL:O	1:A:157:MET:HB3	2.17	0.45
2:C:352:HOH:O	1:D:214:ARG:HD2	2.16	0.45
1:D:188:GLU:OE2	1:D:188:GLU:N	2.46	0.45
1:G:64:TYR:CE2	1:G:66:GLN:HB2	2.51	0.45
1:B:233:VAL:HA	1:C:41:ALA:HA	1.98	0.45
1:B:76:TYR:CZ	1:B:96:THR:HA	2.52	0.44
1:A:51:TYR:O	1:G:55:ILE:HD11	2.17	0.44
1:B:73:GLN:NE2	2:B:303:HOH:O	2.51	0.44
1:D:114:THR:OG1	1:D:115:THR:N	2.48	0.44
1:C:183:MET:O	1:C:186:LEU:HB2	2.18	0.44
1:C:102:THR:HG22	1:C:208:ILE:HD11	2.00	0.44
1:F:232:LYS:HB2	1:F:232:LYS:HE2	1.69	0.43
1:A:186:LEU:HD11	2:A:418:HOH:O	2.17	0.43
1:D:51:TYR:C	1:F:55:ILE:HD11	2.38	0.43
1:B:231:LYS:NZ	1:C:45:GLU:OE1	2.42	0.43
1:A:191:ARG:NH2	2:A:322:HOH:O	2.52	0.43
1:B:183:MET:O	1:B:186:LEU:HB2	2.19	0.43
1:B:229:ARG:HE	1:B:229:ARG:HB3	1.25	0.43
1:C:76:TYR:CZ	1:C:96:THR:HA	2.54	0.43
1:C:162:ARG:NH1	2:C:312:HOH:O	2.50	0.43
1:B:64:TYR:CZ	1:B:66:GLN:HB2	2.54	0.43
1:B:157:MET:O	1:B:161:VAL:HG12	2.18	0.43
1:F:101:SER:OG	1:G:101:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:HA	2:A:320:HOH:O	2.18	0.42
1:G:55:ILE:HD12	1:G:55:ILE:N	2.34	0.42
1:B:23:ARG:NH2	2:B:310:HOH:O	2.33	0.42
1:G:58:MET:HG2	1:G:84:LEU:HD13	2.02	0.42
1:B:79:HIS:HB3	1:C:51:TYR:CE1	2.54	0.42
1:C:149:LEU:HD23	1:C:156:ALA:HB1	2.01	0.42
1:D:21:GLN:HG3	1:D:184:ALA:HB1	2.02	0.42
1:D:236:TRP:O	2:D:304:HOH:O	2.21	0.42
1:A:21:GLN:HG3	1:A:184:ALA:HB1	2.02	0.42
1:B:146:VAL:HG22	1:B:180:CYS:SG	2.59	0.42
1:F:152:ASP:OD2	2:F:305:HOH:O	2.22	0.42
1:A:194:THR:OG1	1:A:196:VAL:HG22	2.19	0.42
1:C:61:VAL:HG11	1:C:88:LEU:HD11	2.02	0.41
1:A:214:ARG:NH2	2:A:313:HOH:O	2.32	0.41
1:B:229:ARG:HA	1:B:230:PRO:HD3	1.95	0.41
1:A:75:GLY:O	1:A:78:GLU:OE1	2.39	0.41
1:A:60:ARG:HA	1:A:60:ARG:HD2	1.82	0.41
1:C:151:GLU:HG2	2:C:344:HOH:O	2.21	0.41
1:G:216:GLY:HA2	2:G:336:HOH:O	2.20	0.41
1:F:189:GLN:CG	2:F:303:HOH:O	2.65	0.41
1:G:191:ARG:HH11	1:G:191:ARG:HG2	1.85	0.41
1:D:229:ARG:HA	1:D:230:PRO:HD3	1.93	0.41
1:G:45:GLU:N	1:G:49:GLU:OE1	2.40	0.41
1:C:42:GLU:HG3	1:C:147:LEU:HD11	2.04	0.40
1:B:102:THR:HG22	1:B:208:ILE:HD11	2.03	0.40
1:G:229:ARG:HA	1:G:230:PRO:HD3	1.90	0.40
1:B:232:LYS:HE2	1:C:42:GLU:OE1	2.22	0.40
1:B:60:ARG:HA	1:B:60:ARG:HD2	1.90	0.40
1:B:157:MET:CE	1:B:186:LEU:HG	2.52	0.40

All (2) 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)
2:F:433:HOH:O	2:G:344:HOH:O[1_655]	1.98	0.22
2:B:310:HOH:O	2:F:394:HOH:O[2_554]	1.99	0.21

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	234/242 (97%)	228 (97%)	6 (3%)	0	100	100
1	B	233/242 (96%)	227 (97%)	6 (3%)	0	100	100
1	C	234/242 (97%)	228 (97%)	6 (3%)	0	100	100
1	D	234/242 (97%)	225 (96%)	8 (3%)	1 (0%)	34	32
1	F	235/242 (97%)	229 (97%)	6 (3%)	0	100	100
1	G	233/242 (96%)	227 (97%)	6 (3%)	0	100	100
All	All	1403/1452 (97%)	1364 (97%)	38 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	235	GLY

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	185/189 (98%)	174 (94%)	11 (6%)	19	17
1	B	184/189 (97%)	170 (92%)	14 (8%)	13	10
1	C	185/189 (98%)	175 (95%)	10 (5%)	22	20
1	D	185/189 (98%)	172 (93%)	13 (7%)	15	12
1	F	186/189 (98%)	173 (93%)	13 (7%)	15	12
1	G	184/189 (97%)	170 (92%)	14 (8%)	13	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1109/1134 (98%)	1034 (93%)	75 (7%)	16	13

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	78	GLU
1	A	84	LEU
1	A	93	VAL
1	A	102	THR
1	A	144	MET
1	A	148	GLU
1	A	187	ASP
1	A	189	GLN
1	A	229	ARG
1	A	233	VAL
1	B	65	ASP
1	B	76	TYR
1	B	84	LEU
1	B	93	VAL
1	B	102	THR
1	B	144	MET
1	B	148	GLU
1	B	161	VAL
1	B	175	VAL
1	B	186	LEU
1	B	187	ASP
1	B	189	GLN
1	B	229	ARG
1	B	233	VAL
1	C	76	TYR
1	C	84	LEU
1	C	93	VAL
1	C	102	THR
1	C	134	GLN
1	C	144	MET
1	C	186	LEU
1	C	189	GLN
1	C	229	ARG
1	C	233	VAL
1	D	6	VAL
1	D	60	ARG

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Mol	Chain	Res	Type
1	D	84	LEU
1	D	93	VAL
1	D	102	THR
1	D	134	GLN
1	D	144	MET
1	D	175	VAL
1	D	187	ASP
1	D	191	ARG
1	D	229	ARG
1	D	233	VAL
1	D	236	TRP
1	F	4	LEU
1	F	84	LEU
1	F	93	VAL
1	F	102	THR
1	F	122	LEU
1	F	144	MET
1	F	148	GLU
1	F	149	LEU
1	F	151	GLU
1	F	186	LEU
1	F	187	ASP
1	F	229	ARG
1	F	233	VAL
1	G	4	LEU
1	G	8	VAL
1	G	84	LEU
1	G	93	VAL
1	G	102	THR
1	G	112	VAL
1	G	129	LEU
1	G	144	MET
1	G	154	VAL
1	G	161	VAL
1	G	175	VAL
1	G	187	ASP
1	G	229	ARG
1	G	233	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	F	134	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 monosaccharides 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	236/242 (97%)	0.49	22 (9%) 8 11	8, 18, 49, 82	0
1	B	235/242 (97%)	-0.03	5 (2%) 63 68	9, 18, 33, 43	0
1	C	236/242 (97%)	0.01	9 (3%) 40 46	7, 16, 33, 52	0
1	D	236/242 (97%)	-0.05	8 (3%) 45 51	6, 14, 35, 51	0
1	F	237/242 (97%)	-0.02	7 (2%) 50 56	8, 17, 33, 46	0
1	G	235/242 (97%)	0.50	28 (11%) 4 5	7, 18, 45, 60	0
All	All	1415/1452 (97%)	0.15	79 (5%) 24 29	6, 17, 38, 82	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	ALA	11.8
1	A	180	CYS	10.8
1	A	149	LEU	9.3
1	G	145	ALA	9.0
1	A	146	VAL	7.9
1	A	144	MET	7.6
1	A	186	LEU	7.6
1	G	146	VAL	7.5
1	A	185	GLY	7.3
1	A	147	LEU	7.2
1	G	147	LEU	7.0
1	G	180	CYS	6.7
1	A	153	PRO	6.5
1	A	151	GLU	6.3
1	D	236	TRP	6.0
1	C	236	TRP	5.6
1	G	144	MET	5.3
1	A	236	TRP	5.3
1	A	148	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	76	TYR	5.0
1	D	184	ALA	5.0
1	A	184	ALA	4.9
1	G	149	LEU	4.8
1	B	76	TYR	4.7
1	G	153	PRO	4.7
1	A	152	ASP	4.4
1	C	232	LYS	4.2
1	G	185	GLY	4.2
1	G	186	LEU	4.1
1	G	148	GLU	4.0
1	G	151	GLU	4.0
1	C	235	GLY	3.9
1	G	229	ARG	3.8
1	D	150	GLU	3.8
1	A	182	GLY	3.8
1	C	151	GLU	3.7
1	G	154	VAL	3.7
1	A	150	GLU	3.7
1	C	233	VAL	3.6
1	G	152	ASP	3.6
1	A	181	GLY	3.5
1	C	76	TYR	3.1
1	B	229	ARG	3.0
1	D	149	LEU	3.0
1	G	182	GLY	3.0
1	D	182	GLY	2.9
1	G	184	ALA	2.9
1	A	235	GLY	2.8
1	F	193	ARG	2.8
1	G	232	LYS	2.8
1	F	180	CYS	2.8
1	G	181	GLY	2.7
1	G	156	ALA	2.7
1	G	188	GLU	2.6
1	A	157	MET	2.6
1	F	186	LEU	2.6
1	G	150	GLU	2.5
1	F	76	TYR	2.4
1	G	65	ASP	2.4
1	B	77	GLY	2.4
1	C	144	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	178	LEU	2.4
1	F	236	TRP	2.4
1	D	66	GLN	2.4
1	G	187	ASP	2.4
1	A	233	VAL	2.3
1	D	151	GLU	2.3
1	F	237	PRO	2.3
1	D	181	GLY	2.3
1	C	148	GLU	2.3
1	A	229	ARG	2.2
1	C	146	VAL	2.2
1	B	235	GLY	2.2
1	F	150	GLU	2.2
1	A	188	GLU	2.1
1	G	192	GLN	2.1
1	G	233	VAL	2.0
1	B	180	CYS	2.0
1	G	157	MET	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 monosaccharides 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.