



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:39 PM UTC

PDB ID : 4U6U / pdb_00004u6u
Title : Crystal Structure of the Cog5-Cog7 complex from Kluyveromyces lactis
Authors : Ha, J.Y.; Jeffrey, P.D.; Hughson, F.M.
Deposited on : 2014-07-29
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

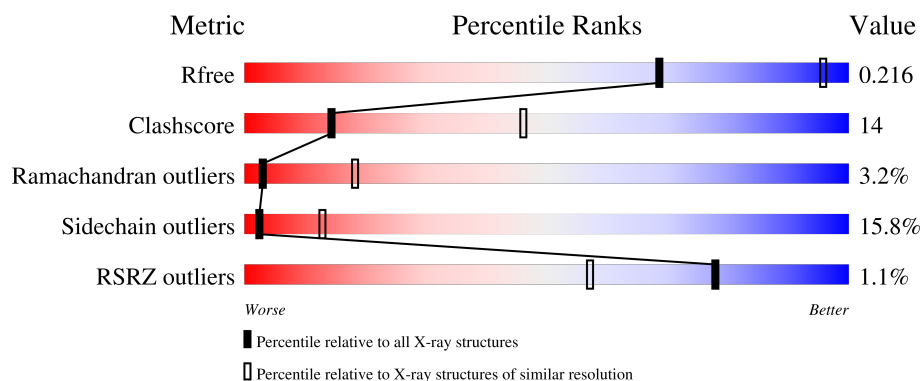
1 Overall quality at a glance

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	77	8% 45% 29% 13% 13%
1	C	77	% 48% 31% 8% 13%
2	B	290	57% 29% 10% ..
2	D	290	63% 27% 8% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5507 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 Cog7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			536	343	80	110	3			
1	C	67	Total	C	N	O	S	0	0	0
			532	340	79	110	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP Q6CXE9
C	4	MET	-	initiating methionine	UNP Q6CXE9

- Molecule 2 is a protein called Cog5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	282	Total	C	N	O	S	0	0	0
			2216	1388	383	433	12			
2	D	283	Total	C	N	O	S	0	0	0
			2223	1392	384	435	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	GLY	-	expression tag	UNP Q6CLE2
B	157	ALA	GLU	engineered mutation	UNP Q6CLE2
B	158	ALA	GLN	engineered mutation	UNP Q6CLE2
B	177	ALA	GLU	engineered mutation	UNP Q6CLE2
B	178	ALA	GLN	engineered mutation	UNP Q6CLE2
B	294	ALA	GLU	engineered mutation	UNP Q6CLE2
B	295	ALA	GLU	engineered mutation	UNP Q6CLE2
B	297	ALA	GLU	engineered mutation	UNP Q6CLE2
D	98	GLY	-	expression tag	UNP Q6CLE2
D	157	ALA	GLU	engineered mutation	UNP Q6CLE2

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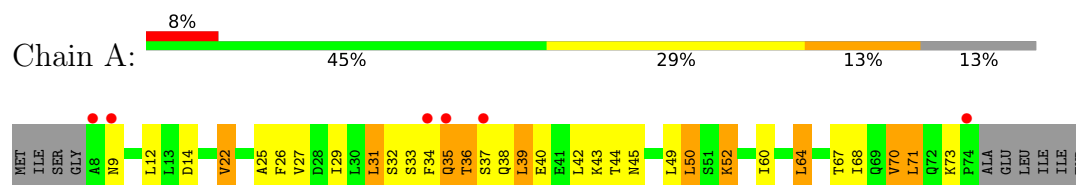
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Chain	Residue	Modelled	Actual	Comment	Reference
D	158	ALA	GLN	engineered mutation	UNP Q6CLE2
D	177	ALA	GLU	engineered mutation	UNP Q6CLE2
D	178	ALA	GLN	engineered mutation	UNP Q6CLE2
D	294	ALA	GLU	engineered mutation	UNP Q6CLE2
D	295	ALA	GLU	engineered mutation	UNP Q6CLE2
D	297	ALA	GLU	engineered mutation	UNP Q6CLE2

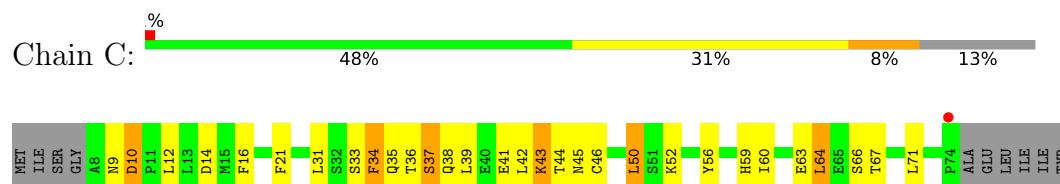
3 Residue-property plots

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.

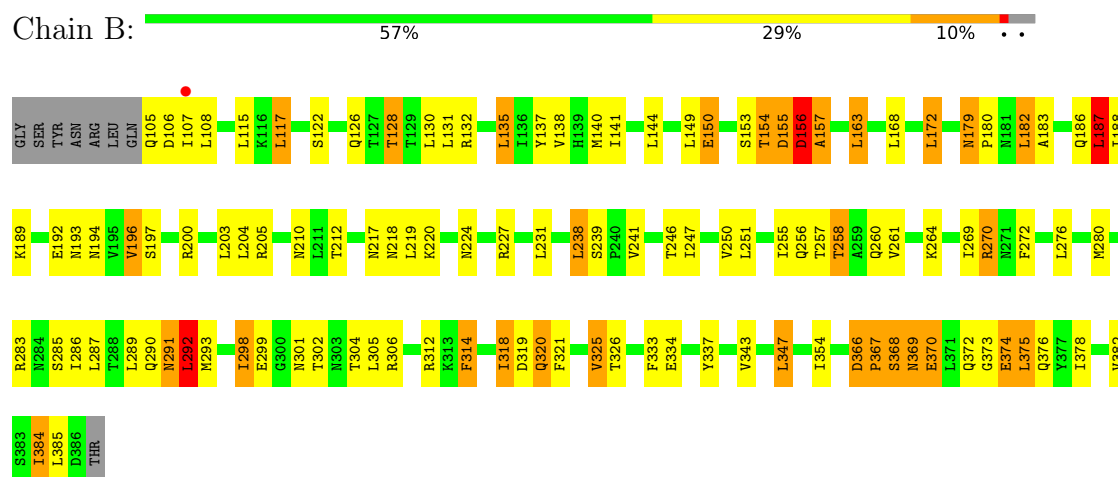
• Molecule 1: Cog7



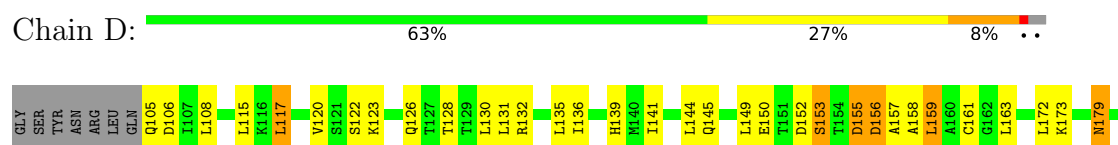
• Molecule 1: Cog7

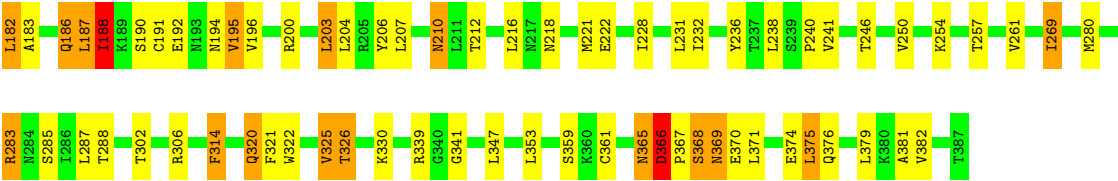


• Molecule 2: Cog5



• Molecule 2: Cog5





4 Data and refinement statistics

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	335.84Å 335.84Å 335.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 3.00 48.47 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.47-3.00) 99.9 (48.47-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.190 , 0.231 (Not available) , 0.216	Depositor DCC
R_{free} test set	2426 reflections (7.35%)	wwPDB-VP
Wilson B-factor (Å ²)	92.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5507	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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	0.67	0/546	1.07	1/739 (0.1%)
1	C	0.63	0/542	1.12	4/735 (0.5%)
2	B	0.56	0/2243	1.07	18/3035 (0.6%)
2	D	0.63	0/2250	1.05	8/3045 (0.3%)
All	All	0.61	0/5581	1.07	31/7554 (0.4%)

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	C	0	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	291	ASN	N-CA-C	10.54	124.84	111.24
1	A	52	LYS	N-CA-C	-9.95	100.69	113.12
1	C	52	LYS	N-CA-C	-8.91	99.21	112.04
2	D	106	ASP	N-CA-C	-8.46	102.96	113.28
2	B	291	ASN	CA-C-N	8.29	136.62	121.70
2	B	291	ASN	C-N-CA	8.29	136.62	121.70
1	C	34	PHE	N-CA-C	7.38	120.90	109.60
2	D	188	ILE	N-CA-C	-6.63	103.00	112.35
2	B	106	ASP	N-CA-C	-6.63	105.08	112.57
2	B	156	ASP	N-CA-C	6.42	124.49	110.80
2	D	186	GLN	N-CA-C	-6.39	101.66	110.35
2	B	156	ASP	CA-C-N	6.33	133.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	156	ASP	C-N-CA	6.33	133.10	121.70
1	C	44	THR	N-CA-C	-6.25	105.15	112.89
2	D	341	GLY	CA-C-N	5.81	125.94	119.32
2	D	341	GLY	C-N-CA	5.81	125.94	119.32
2	B	369	ASN	CB-CA-C	-5.71	108.35	116.34
2	B	239	SER	CA-C-N	5.63	125.74	119.32
2	B	239	SER	C-N-CA	5.63	125.74	119.32
2	B	291	ASN	CA-C-O	-5.44	115.09	120.80
2	B	366	ASP	N-CA-C	5.31	121.55	109.81
2	B	374	GLU	N-CA-C	-5.29	105.68	111.82
2	B	150	GLU	N-CA-C	-5.27	98.44	107.61
1	C	59	HIS	N-CA-C	-5.07	105.64	111.07
2	D	366	ASP	CA-C-N	5.07	125.75	120.12
2	D	366	ASP	C-N-CA	5.07	125.75	120.12
2	B	107	ILE	N-CA-C	-5.06	108.57	113.53
2	B	369	ASN	N-CA-C	5.05	115.47	108.00
2	B	187	LEU	N-CA-C	-5.03	107.10	114.39
2	D	155	ASP	N-CA-C	5.02	116.23	109.11
2	B	205	ARG	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	155	ASP	Peptide
2	B	156	ASP	Peptide
1	C	33	SER	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	536	0	520	21	0
1	C	532	0	509	16	0
2	B	2216	0	2270	78	0
2	D	2223	0	2277	57	0
All	All	5507	0	5576	156	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 14.

All (156) 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)
2:B:334:GLU:HG2	2:B:384:ILE:HD12	1.50	0.90
2:B:384:ILE:H	2:B:384:ILE:HD13	1.48	0.78
2:D:183:ALA:HA	2:D:188:ILE:HD11	1.64	0.78
2:B:382:VAL:HG12	2:B:385:LEU:HD21	1.71	0.72
1:A:36:THR:O	1:A:38:GLN:N	2.22	0.72
2:B:368:SER:OG	2:B:369:ASN:N	2.22	0.71
2:B:298:ILE:HG22	2:B:299:GLU:H	1.58	0.68
2:B:333:PHE:CD2	2:B:384:ILE:HD11	2.29	0.68
2:B:193:ASN:HA	2:B:197:SER:HB3	1.75	0.67
2:D:369:ASN:HD22	2:D:371:LEU:H	1.43	0.66
1:A:9:ASN:OD1	1:C:9:ASN:ND2	2.29	0.66
2:D:187:LEU:HA	2:D:190:SER:HB2	1.78	0.65
2:D:155:ASP:O	2:D:157:ALA:N	2.30	0.64
1:A:35:GLN:NE2	2:B:194:ASN:HD22	1.96	0.64
1:A:33:SER:H	1:A:34:PHE:HA	1.63	0.64
1:A:35:GLN:HE22	2:B:194:ASN:HD22	1.43	0.63
2:D:105:GLN:HA	2:D:108:LEU:HB2	1.80	0.63
2:B:314:PHE:CD1	2:B:320:GLN:HG3	2.35	0.62
2:B:333:PHE:HD2	2:B:384:ILE:HD11	1.64	0.61
1:A:32:SER:HA	2:B:187:LEU:HG	1.82	0.61
2:D:322:TRP:O	2:D:326:THR:HB	2.01	0.60
2:B:140:MET:HE3	2:B:172:LEU:HD13	1.84	0.60
2:B:217:ASN:O	2:B:219:LEU:N	2.28	0.60
1:C:41:GLU:O	1:C:43:LYS:N	2.36	0.59
2:D:302:THR:HG22	2:D:306:ARG:NH1	2.17	0.59
2:D:236:TYR:CE1	2:D:240:PRO:HB3	2.37	0.59
2:D:314:PHE:CD1	2:D:320:GLN:HG3	2.38	0.58
1:A:50:LEU:HD13	2:B:131:LEU:HD23	1.85	0.58
2:D:321:PHE:O	2:D:325:VAL:HG13	2.04	0.57
1:C:35:GLN:HG3	2:D:194:ASN:HD22	1.69	0.57
2:B:314:PHE:CD1	2:B:314:PHE:N	2.72	0.57
2:D:132:ARG:O	2:D:136:ILE:HG13	2.05	0.57
2:B:375:LEU:O	2:B:378:ILE:HG22	2.04	0.57
2:B:385:LEU:HD22	2:B:385:LEU:H	1.70	0.56
2:B:212:THR:HG22	2:B:250:VAL:HG23	1.88	0.56
2:B:354:ILE:HG21	2:B:382:VAL:HG11	1.87	0.56
2:D:206:TYR:O	2:D:210:ASN:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:GLU:HA	2:B:196:VAL:HG13	1.89	0.54
2:B:154:THR:O	2:B:154:THR:OG1	2.26	0.54
2:B:156:ASP:N	2:B:157:ALA:HB3	2.22	0.54
2:B:179:ASN:O	2:B:182:LEU:HB2	2.08	0.54
2:D:149:LEU:HG	2:D:150:GLU:H	1.73	0.54
2:D:375:LEU:HD22	2:D:379:LEU:HG	1.90	0.54
1:A:33:SER:N	1:A:34:PHE:HA	2.22	0.53
2:B:224:ASN:HB3	2:B:227:ARG:HB3	1.90	0.53
2:B:150:GLU:HG3	2:B:153:SER:OG	2.09	0.53
2:B:272:PHE:CE2	2:B:276:LEU:HD22	2.44	0.53
2:B:321:PHE:O	2:B:325:VAL:HG13	2.08	0.53
2:B:155:ASP:C	2:B:157:ALA:HB3	2.34	0.53
2:B:302:THR:HG22	2:B:306:ARG:HH11	1.74	0.53
2:D:314:PHE:CD1	2:D:314:PHE:N	2.76	0.53
2:B:314:PHE:CG	2:B:320:GLN:HG3	2.44	0.52
2:B:217:ASN:C	2:B:219:LEU:H	2.17	0.52
2:B:366:ASP:HA	2:B:372:GLN:NE2	2.24	0.52
2:D:192:GLU:HA	2:D:196:VAL:HG22	1.90	0.52
1:A:33:SER:O	1:A:33:SER:OG	2.26	0.51
2:D:141:ILE:O	2:D:145:GLN:HG2	2.11	0.51
2:D:182:LEU:HD22	2:D:188:ILE:HD13	1.93	0.51
2:B:289:LEU:O	2:B:292:LEU:HB3	2.11	0.50
1:A:64:LEU:HG	2:B:117:LEU:HB3	1.92	0.50
2:B:105:GLN:HB3	2:B:108:LEU:HG	1.94	0.49
2:D:179:ASN:O	2:D:182:LEU:HB2	2.12	0.49
1:A:67:THR:O	1:A:70:VAL:HG22	2.13	0.49
2:B:122:SER:O	2:B:126:GLN:HG3	2.13	0.49
1:C:35:GLN:CG	2:D:194:ASN:HD22	2.26	0.49
2:B:280:MET:HA	2:B:283:ARG:HB3	1.95	0.49
2:D:212:THR:HG23	2:D:246:THR:HG23	1.94	0.49
2:D:122:SER:O	2:D:126:GLN:HG3	2.12	0.48
2:D:359:SER:C	2:D:361:CYS:H	2.21	0.48
2:D:283:ARG:HE	2:D:374:GLU:CD	2.22	0.48
2:B:212:THR:HG23	2:B:246:THR:HG23	1.95	0.48
1:A:52:LYS:HE2	1:C:66:SER:OG	2.14	0.48
1:C:35:GLN:H	1:C:35:GLN:CD	2.22	0.48
2:B:183:ALA:O	2:B:189:LYS:HE2	2.15	0.47
2:B:301:ASN:CG	2:B:302:THR:H	2.23	0.47
1:C:46:CYS:O	1:C:50:LEU:HB2	2.14	0.47
2:D:314:PHE:CG	2:D:320:GLN:HG3	2.49	0.47
2:B:372:GLN:HG2	2:B:373:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:ARG:HD2	2:B:314:PHE:CE2	2.51	0.46
2:D:314:PHE:HB3	2:D:320:GLN:HG3	1.97	0.46
2:B:290:GLN:O	2:B:305:LEU:HD22	2.16	0.46
1:C:21:PHE:HD2	2:D:123:LYS:HD3	1.80	0.46
2:B:260:GLN:HG2	2:B:264:LYS:HE3	1.98	0.46
2:D:283:ARG:NE	2:D:374:GLU:OE2	2.44	0.46
1:A:27:VAL:HG12	1:A:31:LEU:HD22	1.98	0.46
2:B:163:LEU:HD12	2:B:163:LEU:HA	1.80	0.46
2:D:156:ASP:N	2:D:156:ASP:OD1	2.49	0.46
2:D:191:CYS:O	2:D:195:VAL:HG23	2.16	0.46
2:D:366:ASP:HA	2:D:367:PRO:HD3	1.75	0.45
2:B:347:LEU:HD12	2:B:347:LEU:HA	1.78	0.45
2:D:228:ILE:O	2:D:232:ILE:HG13	2.17	0.45
2:D:212:THR:HG22	2:D:250:VAL:HG23	1.98	0.45
2:B:149:LEU:HG	2:B:150:GLU:H	1.81	0.45
2:B:204:LEU:HD22	2:B:238:LEU:HD13	1.98	0.45
1:A:40:GLU:O	1:A:44:THR:HG23	2.16	0.45
1:C:63:GLU:O	1:C:67:THR:HG23	2.16	0.45
2:B:258:THR:O	2:B:261:VAL:HG12	2.17	0.44
1:A:35:GLN:CD	1:A:36:THR:HG23	2.42	0.44
2:B:291:ASN:HB2	2:B:292:LEU:HB2	2.00	0.44
2:B:366:ASP:HB2	2:B:367:PRO:HD3	2.00	0.44
2:B:196:VAL:O	2:B:200:ARG:HB2	2.18	0.44
2:B:286:ILE:HG22	2:B:318:ILE:HD12	2.00	0.44
1:C:16:PHE:HB3	2:D:120:VAL:HG13	1.98	0.44
2:D:158:ALA:HA	2:D:161:CYS:HB3	2.00	0.44
2:D:368:SER:OG	2:D:369:ASN:N	2.51	0.44
2:B:366:ASP:OD1	2:B:372:GLN:NE2	2.51	0.43
2:B:369:ASN:HB3	2:B:370:GLU:H	1.42	0.43
2:D:330:LYS:HB2	2:D:381:ALA:HA	1.99	0.43
2:B:251:LEU:O	2:B:255:ILE:HG23	2.18	0.43
2:B:299:GLU:O	2:B:301:ASN:N	2.51	0.43
2:B:337:TYR:CG	2:B:384:ILE:HG13	2.54	0.43
2:D:216:LEU:HA	2:D:254:LYS:NZ	2.34	0.43
2:B:128:THR:HG23	2:B:132:ARG:NH1	2.34	0.43
2:B:293:MET:O	2:B:304:THR:OG1	2.29	0.43
2:D:280:MET:HG3	2:D:361:CYS:SG	2.59	0.43
1:A:22:VAL:HG22	1:A:25:ALA:H	1.84	0.43
2:B:270:ARG:NH1	2:B:270:ARG:HB2	2.34	0.43
2:D:218:ASN:O	2:D:221:MET:HB3	2.19	0.43
2:B:137:TYR:O	2:B:140:MET:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:ASP:HA	2:B:372:GLN:CD	2.43	0.43
2:D:179:ASN:HD22	2:D:179:ASN:HA	1.66	0.43
1:A:26:PHE:O	1:A:29:ILE:HG12	2.18	0.43
2:B:373:GLY:HA2	2:B:376:GLN:OE1	2.19	0.43
2:B:280:MET:SD	2:B:283:ARG:HG2	2.59	0.42
2:B:155:ASP:O	2:B:157:ALA:HB3	2.19	0.42
2:B:385:LEU:HD22	2:B:385:LEU:N	2.33	0.42
2:D:150:GLU:HG2	2:D:153:SER:OG	2.19	0.42
2:D:186:GLN:O	2:D:187:LEU:HB3	2.19	0.42
2:D:365:ASN:HB3	2:D:366:ASP:H	1.76	0.42
2:B:283:ARG:NE	2:B:374:GLU:OE1	2.51	0.42
2:D:269:ILE:H	2:D:269:ILE:HG13	1.56	0.42
1:A:43:LYS:HD3	2:B:138:VAL:HG12	2.01	0.42
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.79	0.42
2:D:280:MET:HE3	2:D:280:MET:HB3	1.78	0.42
1:A:27:VAL:HG13	2:B:131:LEU:HD13	2.01	0.42
2:D:254:LYS:HE3	2:D:285:SER:OG	2.19	0.42
2:D:173:LYS:HE2	2:D:200:ARG:HH21	1.83	0.42
2:D:157:ALA:C	2:D:159:LEU:H	2.28	0.42
2:D:203:LEU:HD22	2:D:207:LEU:HG	2.02	0.41
1:C:64:LEU:HD23	1:C:64:LEU:HA	1.74	0.41
2:D:173:LYS:CE	2:D:200:ARG:HE	2.33	0.41
2:B:204:LEU:HD21	2:B:238:LEU:HD22	2.01	0.41
2:D:187:LEU:O	2:D:187:LEU:HD13	2.20	0.41
2:B:179:ASN:HA	2:B:180:PRO:HD2	1.84	0.41
1:A:39:LEU:HD23	2:B:138:VAL:HG13	2.03	0.41
1:C:64:LEU:HG	2:D:117:LEU:HB3	2.02	0.41
1:C:10:ASP:OD1	1:C:12:LEU:HB3	2.20	0.41
2:B:298:ILE:HG22	2:B:299:GLU:N	2.32	0.41
1:C:43:LYS:HE2	2:D:139:HIS:NE2	2.36	0.41
2:D:222:GLU:OE1	2:D:288:THR:HG21	2.20	0.41
1:A:68:ILE:O	1:A:71:LEU:HB2	2.21	0.41
2:D:117:LEU:HD12	2:D:117:LEU:HA	1.87	0.41
2:B:217:ASN:OD1	2:B:220:LYS:HG2	2.22	0.40
1:C:37:SER:OG	1:C:38:GLN:N	2.52	0.40
2:B:292:LEU:HD22	2:B:292:LEU:HA	1.71	0.40
1:C:12:LEU:HD23	1:C:56:TYR:HE2	1.87	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	65/77 (84%)	56 (86%)	6 (9%)	3 (5%)	2	11
1	C	65/77 (84%)	53 (82%)	8 (12%)	4 (6%)	1	6
2	B	280/290 (97%)	253 (90%)	19 (7%)	8 (3%)	3	20
2	D	281/290 (97%)	253 (90%)	21 (8%)	7 (2%)	4	23
All	All	691/734 (94%)	615 (89%)	54 (8%)	22 (3%)	3	18

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	37	SER
2	B	156	ASP
2	B	368	SER
2	B	370	GLU
1	C	36	THR
1	C	37	SER
2	D	368	SER
2	B	186	GLN
2	B	218	ASN
2	B	367	PRO
1	C	43	LYS
2	D	152	ASP
2	D	153	SER
2	D	370	GLU
2	B	292	LEU
2	D	365	ASN
1	A	73	LYS
2	B	157	ALA
1	C	34	PHE
2	D	187	LEU
2	D	366	ASP

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	64/72 (89%)	50 (78%)	14 (22%)	1	5
1	C	63/72 (88%)	53 (84%)	10 (16%)	2	13
2	B	258/265 (97%)	217 (84%)	41 (16%)	2	13
2	D	259/265 (98%)	222 (86%)	37 (14%)	3	16
All	All	644/674 (96%)	542 (84%)	102 (16%)	2	13

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	14	ASP
1	A	22	VAL
1	A	31	LEU
1	A	35	GLN
1	A	39	LEU
1	A	42	LEU
1	A	45	ASN
1	A	49	LEU
1	A	50	LEU
1	A	60	ILE
1	A	64	LEU
1	A	70	VAL
1	A	71	LEU
2	B	115	LEU
2	B	117	LEU
2	B	128	THR
2	B	130	LEU
2	B	135	LEU
2	B	141	ILE
2	B	144	LEU
2	B	154	THR
2	B	163	LEU
2	B	168	LEU

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Mol	Chain	Res	Type
2	B	172	LEU
2	B	179	ASN
2	B	182	LEU
2	B	187	LEU
2	B	188	ILE
2	B	196	VAL
2	B	203	LEU
2	B	210	ASN
2	B	231	LEU
2	B	238	LEU
2	B	241	VAL
2	B	247	ILE
2	B	256	GLN
2	B	257	THR
2	B	258	THR
2	B	269	ILE
2	B	270	ARG
2	B	285	SER
2	B	287	LEU
2	B	292	LEU
2	B	298	ILE
2	B	314	PHE
2	B	318	ILE
2	B	319	ASP
2	B	320	GLN
2	B	325	VAL
2	B	326	THR
2	B	343	VAL
2	B	347	LEU
2	B	375	LEU
2	B	384	ILE
1	C	10	ASP
1	C	14	ASP
1	C	31	LEU
1	C	39	LEU
1	C	42	LEU
1	C	45	ASN
1	C	50	LEU
1	C	60	ILE
1	C	64	LEU
1	C	71	LEU
2	D	115	LEU

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Mol	Chain	Res	Type
2	D	117	LEU
2	D	128	THR
2	D	130	LEU
2	D	131	LEU
2	D	135	LEU
2	D	144	LEU
2	D	156	ASP
2	D	159	LEU
2	D	163	LEU
2	D	172	LEU
2	D	179	ASN
2	D	182	LEU
2	D	188	ILE
2	D	195	VAL
2	D	203	LEU
2	D	204	LEU
2	D	210	ASN
2	D	231	LEU
2	D	238	LEU
2	D	241	VAL
2	D	257	THR
2	D	261	VAL
2	D	269	ILE
2	D	283	ARG
2	D	287	LEU
2	D	314	PHE
2	D	320	GLN
2	D	325	VAL
2	D	326	THR
2	D	339	ARG
2	D	347	LEU
2	D	353	LEU
2	D	369	ASN
2	D	375	LEU
2	D	376	GLN
2	D	382	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
2	B	179	ASN

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Mol	Chain	Res	Type
2	B	194	ASN
2	B	290	GLN
2	B	372	GLN
2	D	179	ASN
2	D	194	ASN
2	D	348	GLN
2	D	369	ASN
2	D	376	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	67/77 (87%)	-0.05	6 (8%) 15 8	51, 92, 186, 247	0
1	C	67/77 (87%)	-0.27	1 (1%) 72 49	55, 99, 182, 234	0
2	B	282/290 (97%)	-0.19	1 (0%) 88 76	50, 130, 183, 257	0
2	D	283/290 (97%)	-0.43	0 100 100	57, 86, 151, 245	0
All	All	699/734 (95%)	-0.28	8 (1%) 78 57	50, 107, 180, 257	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	5.5
1	A	74	PRO	3.1
1	C	74	PRO	2.6
1	A	37	SER	2.4
1	A	35	GLN	2.4
2	B	107	ILE	2.2
1	A	9	ASN	2.2
1	A	34	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.