



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:09 AM UTC

PDB ID : 4GML / pdb_00004gml
Title : Crystal structure of human NOT1 MIF4G domain
Authors : Petit, P.; Weichenrieder, O.; Wohlbold, L.; Izaurralde, E.
Deposited on : 2012-08-16
Resolution : 2.90 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

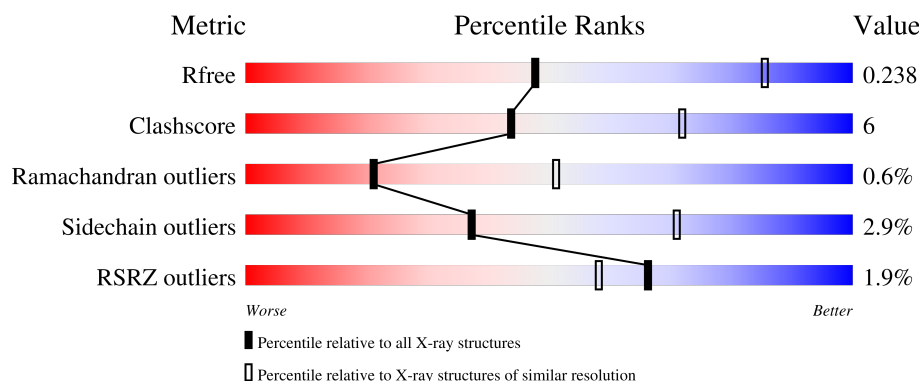
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	235	2% 88% 10% .
1	B	235	% 81% 18% .
1	C	235	% 78% 14% 5% .
1	D	235	3% 87% 12% .
1	E	235	2% 83% 12% .

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Mol	Chain	Length	Quality of chain
1	F	235	3% 77% 21% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11132 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 CCR4-NOT transcription complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1896	1224	315	348	9			
1	B	235	Total	C	N	O	S	0	0	0
			1893	1222	315	347	9			
1	C	223	Total	C	N	O	S	0	0	0
			1786	1154	293	331	8			
1	D	233	Total	C	N	O	S	0	0	0
			1871	1207	312	343	9			
1	E	226	Total	C	N	O	S	0	0	0
			1811	1166	301	336	8			
1	F	233	Total	C	N	O	S	0	0	0
			1845	1190	306	340	9			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	VAL	-	expression tag	UNP A5YKK6
A	-8	LEU	-	expression tag	UNP A5YKK6
A	-7	PHE	-	expression tag	UNP A5YKK6
A	-6	GLN	-	expression tag	UNP A5YKK6
A	-5	GLY	-	expression tag	UNP A5YKK6
A	-4	PRO	-	expression tag	UNP A5YKK6
A	-3	HIS	-	expression tag	UNP A5YKK6
A	-2	MET	-	expression tag	UNP A5YKK6
A	-1	LEU	-	expression tag	UNP A5YKK6
A	0	GLU	-	expression tag	UNP A5YKK6
B	-9	VAL	-	expression tag	UNP A5YKK6
B	-8	LEU	-	expression tag	UNP A5YKK6
B	-7	PHE	-	expression tag	UNP A5YKK6
B	-6	GLN	-	expression tag	UNP A5YKK6
B	-5	GLY	-	expression tag	UNP A5YKK6
B	-4	PRO	-	expression tag	UNP A5YKK6
B	-3	HIS	-	expression tag	UNP A5YKK6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP A5YKK6
B	-1	LEU	-	expression tag	UNP A5YKK6
B	0	GLU	-	expression tag	UNP A5YKK6
C	-9	VAL	-	expression tag	UNP A5YKK6
C	-8	LEU	-	expression tag	UNP A5YKK6
C	-7	PHE	-	expression tag	UNP A5YKK6
C	-6	GLN	-	expression tag	UNP A5YKK6
C	-5	GLY	-	expression tag	UNP A5YKK6
C	-4	PRO	-	expression tag	UNP A5YKK6
C	-3	HIS	-	expression tag	UNP A5YKK6
C	-2	MET	-	expression tag	UNP A5YKK6
C	-1	LEU	-	expression tag	UNP A5YKK6
C	0	GLU	-	expression tag	UNP A5YKK6
D	-9	VAL	-	expression tag	UNP A5YKK6
D	-8	LEU	-	expression tag	UNP A5YKK6
D	-7	PHE	-	expression tag	UNP A5YKK6
D	-6	GLN	-	expression tag	UNP A5YKK6
D	-5	GLY	-	expression tag	UNP A5YKK6
D	-4	PRO	-	expression tag	UNP A5YKK6
D	-3	HIS	-	expression tag	UNP A5YKK6
D	-2	MET	-	expression tag	UNP A5YKK6
D	-1	LEU	-	expression tag	UNP A5YKK6
D	0	GLU	-	expression tag	UNP A5YKK6
E	-9	VAL	-	expression tag	UNP A5YKK6
E	-8	LEU	-	expression tag	UNP A5YKK6
E	-7	PHE	-	expression tag	UNP A5YKK6
E	-6	GLN	-	expression tag	UNP A5YKK6
E	-5	GLY	-	expression tag	UNP A5YKK6
E	-4	PRO	-	expression tag	UNP A5YKK6
E	-3	HIS	-	expression tag	UNP A5YKK6
E	-2	MET	-	expression tag	UNP A5YKK6
E	-1	LEU	-	expression tag	UNP A5YKK6
E	0	GLU	-	expression tag	UNP A5YKK6
F	-9	VAL	-	expression tag	UNP A5YKK6
F	-8	LEU	-	expression tag	UNP A5YKK6
F	-7	PHE	-	expression tag	UNP A5YKK6
F	-6	GLN	-	expression tag	UNP A5YKK6
F	-5	GLY	-	expression tag	UNP A5YKK6
F	-4	PRO	-	expression tag	UNP A5YKK6
F	-3	HIS	-	expression tag	UNP A5YKK6
F	-2	MET	-	expression tag	UNP A5YKK6
F	-1	LEU	-	expression tag	UNP A5YKK6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLU	-	expression tag	UNP A5YKK6

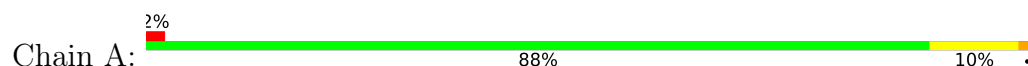
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	6	Total O 6 6	0	0
2	C	4	Total O 4 4	0	0
2	D	8	Total O 8 8	0	0
2	E	1	Total O 1 1	0	0
2	F	2	Total O 2 2	0	0

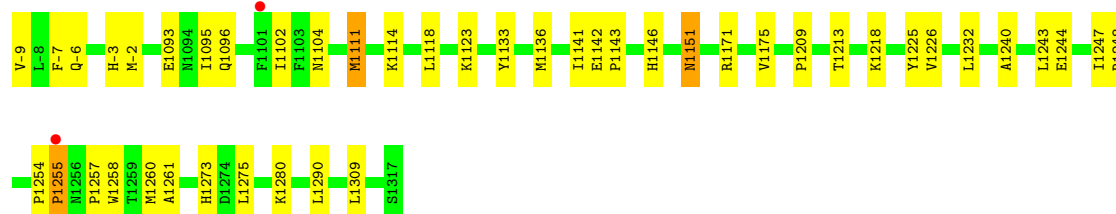
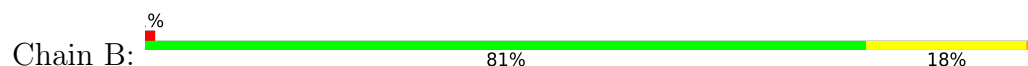
3 Residue-property plots

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.

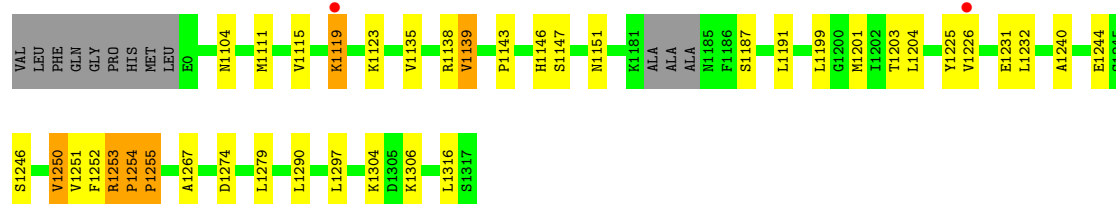
• Molecule 1: CCR4-NOT transcription complex subunit 1



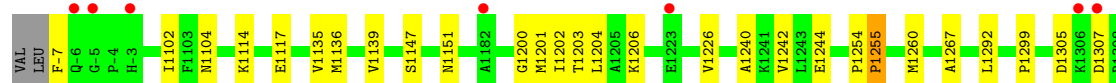
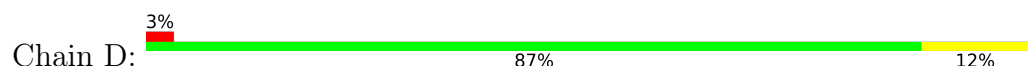
• Molecule 1: CCR4-NOT transcription complex subunit 1



• Molecule 1: CCR4-NOT transcription complex subunit 1

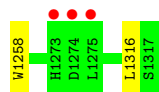
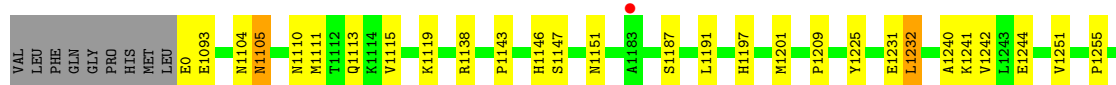
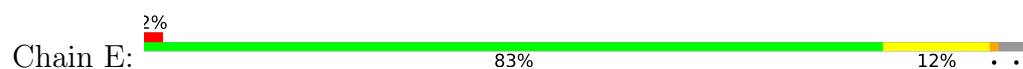


• Molecule 1: CCR4-NOT transcription complex subunit 1

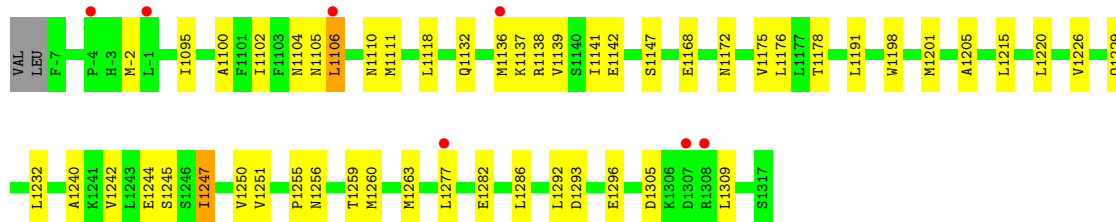
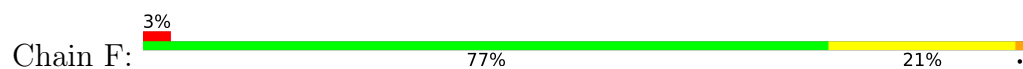




- Molecule 1: CCR4-NOT transcription complex subunit 1



- Molecule 1: CCR4-NOT transcription complex subunit 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.27Å 133.82Å 331.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 2.90 49.31 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.31-2.90) 95.2 (49.31-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.190 , 0.229 0.198 , 0.238	Depositor DCC
R_{free} test set	2216 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 86.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11132	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	0.31	0/1933	0.73	2/2618 (0.1%)
1	B	0.29	0/1930	0.74	0/2615
1	C	0.30	0/1819	0.72	0/2465
1	D	0.30	0/1907	0.70	0/2582
1	E	0.30	0/1845	0.74	0/2501
1	F	0.30	0/1881	0.75	1/2555 (0.0%)
All	All	0.30	0/11315	0.73	3/15336 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1095	ILE	N-CA-C	-7.03	106.64	113.53
1	A	-5	GLY	CA-C-N	5.42	125.24	119.28
1	A	-5	GLY	C-N-CA	5.42	125.24	119.28

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	1896	0	1930	17	0
1	B	1893	0	1923	32	0
1	C	1786	0	1797	26	0
1	D	1871	0	1898	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1811	0	1825	19	0
1	F	1845	0	1840	35	0
2	A	9	0	0	0	0
2	B	6	0	0	0	0
2	C	4	0	0	0	0
2	D	8	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
All	All	11132	0	11213	136	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 6.

All (136) 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:B:1257:PRO:HG2	1:C:1253:ARG:HH21	1.32	0.92
1:D:1203:THR:HG23	1:D:1204:LEU:N	1.82	0.92
1:F:1100:ALA:O	1:F:1104:ASN:HB2	1.73	0.88
1:D:1203:THR:HG23	1:D:1204:LEU:H	1.39	0.87
1:C:1246:SER:HB2	1:C:1252:PHE:O	1.76	0.85
1:F:1139:VAL:HG11	1:F:1198:TRP:CG	2.13	0.83
1:D:1203:THR:CG2	1:D:1204:LEU:H	1.95	0.79
1:B:-2:MET:HE1	1:F:1175:VAL:HG21	1.67	0.76
1:D:1203:THR:CG2	1:D:1204:LEU:N	2.48	0.76
1:D:1104:ASN:O	1:D:1114:LYS:NZ	2.20	0.75
1:B:-3:HIS:HB3	1:F:1191:LEU:HD13	1.71	0.73
1:A:1094:ASN:HB3	1:A:1097:GLU:HB3	1.71	0.72
1:B:1104:ASN:O	1:B:1114:LYS:NZ	2.25	0.69
1:D:1203:THR:HG23	1:D:1204:LEU:HG	1.75	0.68
1:C:1225:TYR:HA	1:C:1232:LEU:HD11	1.76	0.68
1:D:1200:GLY:HA2	1:D:1203:THR:HG22	1.76	0.68
1:F:1102:ILE:HG13	1:F:1118:LEU:HD23	1.77	0.66
1:F:1100:ALA:O	1:F:1104:ASN:CB	2.44	0.64
1:F:1141:ILE:HG13	1:F:1142:GLU:HG3	1.79	0.64
1:B:-9:VAL:HG21	1:B:1133:TYR:HB2	1.80	0.63
1:F:1104:ASN:O	1:F:1105:ASN:HB2	1.98	0.63
1:C:1111:MET:SD	1:C:1151:ASN:ND2	2.73	0.61
1:B:1225:TYR:HA	1:B:1232:LEU:HD11	1.83	0.61
1:B:1258:TRP:HB2	1:C:1250:VAL:HG21	1.83	0.60
1:A:-9:VAL:HG21	1:A:1133:TYR:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1199:LEU:O	1:C:1203:THR:HG22	2.01	0.59
1:B:1141:ILE:HG13	1:B:1142:GLU:HG3	1.84	0.59
1:B:1123:LYS:HE3	1:F:1178:THR:HG21	1.84	0.59
1:D:1260:MET:HE1	1:D:1292:LEU:HD11	1.85	0.58
1:F:1147:SER:HA	1:F:1201:MET:HE1	1.83	0.58
1:B:1257:PRO:HG2	1:C:1253:ARG:NH2	2.12	0.58
1:E:1258:TRP:HB2	1:F:1250:VAL:HG11	1.86	0.57
1:B:1247:ILE:HD11	1:B:1290:LEU:HA	1.87	0.57
1:C:1104:ASN:OD1	1:C:1138:ARG:NH2	2.36	0.57
1:D:1202:ILE:HA	1:D:1206:LYS:HE3	1.87	0.56
1:E:1104:ASN:OD1	1:E:1138:ARG:NH2	2.34	0.56
1:E:1209:PRO:HB3	1:F:1251:VAL:HG21	1.86	0.56
1:F:1215:LEU:HD11	1:F:1220:LEU:HD22	1.87	0.56
1:F:1100:ALA:O	1:F:1104:ASN:N	2.37	0.55
1:F:1205:ALA:HB2	1:F:1245:SER:HB3	1.87	0.55
1:C:1253:ARG:O	1:C:1254:PRO:C	2.50	0.55
1:A:1260:MET:HE1	1:A:1292:LEU:HD11	1.88	0.54
1:F:1106:LEU:HD12	1:F:1110:ASN:OD1	2.07	0.54
1:F:1136:MET:HG2	1:F:1172:ASN:OD1	2.09	0.53
1:C:1203:THR:HG23	1:C:1204:LEU:H	1.74	0.53
1:A:1138:ARG:NH2	1:A:1142:GLU:OE2	2.42	0.53
1:C:1231:GLU:HG2	1:C:1316:LEU:HD13	1.89	0.53
1:E:1111:MET:HE1	1:E:1151:ASN:HB3	1.91	0.52
1:F:1251:VAL:O	1:F:1256:ASN:ND2	2.39	0.52
1:B:1111:MET:SD	1:B:1151:ASN:HB3	2.50	0.52
1:A:-5:GLY:H	1:A:-2:MET:HE2	1.74	0.52
1:B:1254:PRO:HB3	1:B:1260:MET:HE2	1.90	0.52
1:D:1135:VAL:HA	1:D:1139:VAL:HB	1.91	0.52
1:E:1209:PRO:HD3	1:F:1251:VAL:HG11	1.91	0.51
1:A:-6:GLN:HG2	1:A:-2:MET:HE3	1.91	0.51
1:E:1231:GLU:HG2	1:E:1316:LEU:HD13	1.93	0.51
1:A:1183:ALA:O	1:A:1189:ARG:NH2	2.44	0.51
1:E:1225:TYR:HA	1:E:1232:LEU:HD21	1.92	0.51
1:B:1209:PRO:HB3	1:C:1251:VAL:HG21	1.93	0.50
1:B:1093:GLU:HB3	1:B:1095:ILE:HG13	1.93	0.50
1:D:1200:GLY:CA	1:D:1203:THR:HG22	2.42	0.50
1:C:1115:VAL:O	1:C:1119:LYS:HG2	2.11	0.50
1:A:1147:SER:HA	1:A:1201:MET:HE1	1.94	0.50
1:B:1226:VAL:HG11	1:B:1309:LEU:HB3	1.93	0.49
1:D:1114:LYS:HA	1:D:1117:GLU:HG2	1.94	0.49
1:D:1305:ASP:C	1:D:1307:ASP:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1147:SER:HA	1:E:1201:MET:HE1	1.95	0.49
1:B:1275:LEU:O	1:B:1280:LYS:NZ	2.34	0.48
1:B:1275:LEU:HD23	1:B:1280:LYS:HG2	1.95	0.48
1:B:-6:GLN:O	1:F:1137:LYS:NZ	2.46	0.48
1:D:1147:SER:HA	1:D:1201:MET:HE1	1.95	0.48
1:F:1259:THR:O	1:F:1263:MET:HG2	2.13	0.48
1:A:1144:ASN:OD1	1:B:1248:ARG:NH2	2.42	0.48
1:D:1200:GLY:HA2	1:D:1203:THR:CG2	2.43	0.47
1:B:-3:HIS:HB2	1:F:1176:LEU:HD21	1.96	0.47
1:E:1143:PRO:HA	1:E:1146:HIS:CD2	2.49	0.47
1:A:-6:GLN:NE2	1:A:-2:MET:O	2.48	0.47
1:E:1187:SER:O	1:E:1191:LEU:HG	2.15	0.47
1:D:1102:ILE:O	1:D:1114:LYS:HD3	2.15	0.46
1:B:1143:PRO:HA	1:B:1146:HIS:CE1	2.51	0.46
1:D:1267:ALA:HB1	1:D:1299:PRO:HG3	1.98	0.46
1:C:1240:ALA:O	1:C:1244:GLU:HG3	2.16	0.46
1:A:1251:VAL:O	1:A:1256:ASN:ND2	2.33	0.45
1:F:1293:ASP:HB3	1:F:1296:GLU:HB2	1.98	0.45
1:C:1135:VAL:HA	1:C:1139:VAL:HB	1.98	0.45
1:F:1229:GLN:HA	1:F:1232:LEU:HD12	1.99	0.45
1:A:-6:GLN:CG	1:A:-2:MET:HE3	2.47	0.45
1:A:1133:TYR:CZ	1:A:1138:ARG:HD3	2.52	0.45
1:E:1111:MET:HE1	1:E:1151:ASN:C	2.41	0.45
1:B:1254:PRO:HA	1:B:1255:PRO:HA	1.81	0.45
1:C:1203:THR:HG23	1:C:1204:LEU:HG	1.99	0.44
1:E:1197:HIS:HB2	1:E:1241:LYS:HD2	1.99	0.44
1:F:1240:ALA:O	1:F:1244:GLU:HG3	2.18	0.44
1:A:1240:ALA:O	1:A:1244:GLU:HG3	2.17	0.44
1:B:1102:ILE:HG21	1:B:1118:LEU:HB2	2.00	0.44
1:C:1123:LYS:HE2	1:C:1123:LYS:HB3	1.76	0.44
1:C:1254:PRO:HA	1:C:1255:PRO:HA	1.81	0.44
1:F:1139:VAL:CG1	1:F:1198:TRP:HB2	2.47	0.44
1:F:1247:ILE:HD13	1:F:1247:ILE:HA	1.75	0.44
1:E:1115:VAL:O	1:E:1119:LYS:HG3	2.17	0.44
1:F:1201:MET:HE2	1:F:1201:MET:HB3	1.92	0.44
1:A:1181:LYS:NZ	1:A:1317:SER:OG	2.51	0.44
1:E:1111:MET:HE1	1:E:1151:ASN:CB	2.48	0.43
1:E:1240:ALA:O	1:E:1244:GLU:HG3	2.18	0.43
1:C:1253:ARG:O	1:C:1254:PRO:O	2.36	0.43
1:D:1201:MET:HE2	1:D:1201:MET:HB3	1.89	0.43
1:E:1258:TRP:CB	1:F:1250:VAL:HG11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1203:THR:HG23	1:C:1204:LEU:N	2.34	0.43
1:C:1253:ARG:HH11	1:C:1253:ARG:HB2	1.84	0.43
1:D:1240:ALA:O	1:D:1244:GLU:HG3	2.19	0.42
1:D:1254:PRO:HA	1:D:1255:PRO:HA	1.79	0.42
1:B:1218:LYS:HE3	1:B:1261:ALA:HB1	2.01	0.42
1:B:1240:ALA:O	1:B:1244:GLU:HG3	2.19	0.42
1:B:1136:MET:HE2	1:B:1136:MET:HB3	1.94	0.42
1:D:1226:VAL:HG11	1:D:1309:LEU:HB3	2.00	0.42
1:D:1136:MET:HE3	1:D:1136:MET:HB2	1.93	0.42
1:E:1241:LYS:NZ	1:E:1244:GLU:OE2	2.50	0.42
1:B:1243:LEU:HD23	1:B:1243:LEU:HA	1.87	0.42
1:B:-9:VAL:HG13	1:B:1096:GLN:HG3	2.01	0.42
1:F:1226:VAL:HG11	1:F:1309:LEU:HG	2.02	0.42
1:A:1093:GLU:O	1:A:1093:GLU:HG3	2.19	0.42
1:B:-2:MET:HG3	1:F:1136:MET:HE3	2.01	0.41
1:F:1305:ASP:O	1:F:1309:LEU:HB2	2.21	0.41
1:F:1138:ARG:HA	1:F:1138:ARG:HD2	1.96	0.41
1:C:1147:SER:HA	1:C:1201:MET:HE1	2.01	0.41
1:F:1132:GLN:HA	1:F:1168:GLU:HG2	2.02	0.41
1:C:1143:PRO:HA	1:C:1146:HIS:CD2	2.56	0.41
1:A:-8:LEU:HB2	1:A:1132:GLN:OE1	2.21	0.41
1:F:1260:MET:HE1	1:F:1292:LEU:HD11	2.02	0.41
1:B:1171:ARG:O	1:B:1175:VAL:HG23	2.20	0.41
1:C:1304:LYS:O	1:C:1306:LYS:N	2.51	0.41
1:E:1104:ASN:O	1:E:1105:ASN:C	2.64	0.41
1:E:1110:ASN:O	1:E:1113:GLN:HG2	2.21	0.41
1:B:-3:HIS:CD2	1:B:-2:MET:HE3	2.55	0.40
1:C:1187:SER:O	1:C:1191:LEU:HG	2.21	0.40
1:C:1267:ALA:HB2	1:C:1297:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/235 (99%)	226 (97%)	7 (3%)	0	100	100
1	B	233/235 (99%)	224 (96%)	7 (3%)	2 (1%)	14	41
1	C	219/235 (93%)	208 (95%)	9 (4%)	2 (1%)	14	41
1	D	231/235 (98%)	221 (96%)	9 (4%)	1 (0%)	30	59
1	E	224/235 (95%)	214 (96%)	8 (4%)	2 (1%)	14	41
1	F	231/235 (98%)	222 (96%)	8 (4%)	1 (0%)	30	59
All	All	1371/1410 (97%)	1315 (96%)	48 (4%)	8 (1%)	21	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1254	PRO
1	B	-7	PHE
1	E	1105	ASN
1	D	1255	PRO
1	C	1255	PRO
1	B	1255	PRO
1	E	1255	PRO
1	F	1255	PRO

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	215/220 (98%)	207 (96%)	8 (4%)	30	64
1	B	214/220 (97%)	210 (98%)	4 (2%)	50	79
1	C	201/220 (91%)	193 (96%)	8 (4%)	28	62
1	D	210/220 (96%)	207 (99%)	3 (1%)	59	85
1	E	203/220 (92%)	198 (98%)	5 (2%)	42	74
1	F	204/220 (93%)	196 (96%)	8 (4%)	28	63
All	All	1247/1320 (94%)	1211 (97%)	36 (3%)	37	71

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-8	LEU
1	A	1093	GLU
1	A	1141	ILE
1	A	1147	SER
1	A	1187	SER
1	A	1226	VAL
1	A	1250	VAL
1	A	1251	VAL
1	B	1111	MET
1	B	1151	ASN
1	B	1213	THR
1	B	1273	HIS
1	C	1119	LYS
1	C	1139	VAL
1	C	1226	VAL
1	C	1250	VAL
1	C	1253	ARG
1	C	1274	ASP
1	C	1279	LEU
1	C	1290	LEU
1	D	-7	PHE
1	D	1151	ASN
1	D	1242	VAL
1	E	0	GLU
1	E	1093	GLU
1	E	1232	LEU
1	E	1242	VAL
1	E	1251	VAL
1	F	-2	MET
1	F	1106	LEU
1	F	1111	MET
1	F	1242	VAL
1	F	1247	ILE
1	F	1277	LEU
1	F	1282	GLU
1	F	1286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1230	GLN

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Mol	Chain	Res	Type
1	A	1301	ASN
1	C	1273	HIS
1	D	1207	ASN
1	D	1230	GLN
1	D	1270	HIS
1	D	1311	ASN
1	E	1212	HIS
1	F	1096	GLN
1	F	1108	GLN
1	F	1151	ASN
1	F	1311	ASN
1	F	1315	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

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	235/235 (100%)	-0.17	4 (1%) 69 61	44, 66, 104, 123	0
1	B	235/235 (100%)	-0.04	2 (0%) 81 75	49, 71, 112, 142	0
1	C	223/235 (94%)	0.04	2 (0%) 81 75	24, 69, 113, 129	0
1	D	233/235 (99%)	0.08	7 (3%) 52 43	28, 65, 108, 137	0
1	E	226/235 (96%)	0.16	4 (1%) 67 59	55, 79, 119, 152	0
1	F	233/235 (99%)	0.21	7 (3%) 52 43	54, 77, 117, 130	0
All	All	1385/1410 (98%)	0.05	26 (1%) 66 58	24, 72, 115, 152	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	-4	PRO	4.8
1	A	0	GLU	4.0
1	B	1255	PRO	3.1
1	C	1119	LYS	3.0
1	E	1183	ALA	2.9
1	F	1277	LEU	2.8
1	E	1274	ASP	2.8
1	D	1307	ASP	2.8
1	F	1136	MET	2.7
1	D	1306	LYS	2.6
1	E	1273	HIS	2.5
1	D	1223	GLU	2.5
1	D	-6	GLN	2.4
1	D	-5	GLY	2.4
1	C	1226	VAL	2.3
1	B	1101	PHE	2.2
1	F	1106	LEU	2.2
1	F	1308	ARG	2.2
1	A	1093	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	1275	LEU	2.2
1	A	-9	VAL	2.2
1	D	-3	HIS	2.2
1	D	1182	ALA	2.2
1	A	-2	MET	2.1
1	F	-1	LEU	2.1
1	F	1307	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 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.