



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:42 AM EDT

PDB ID : 4CV5 / pdb_00004cv5
Title : yeast NOT1 CN9BD-CAF40 complex
Authors : Basquin, J.; Conti, E.
Deposited on : 2014-03-23
Resolution : 3.81 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

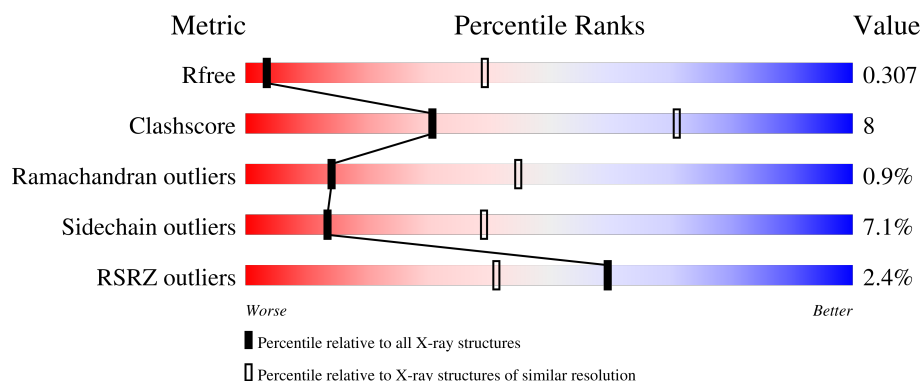
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	212	0% 69% 16% • 13%
1	C	212	2% 69% 17% • 13%
2	B	320	2% 63% 17% • 19%
2	D	320	2% 64% 15% • 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TBR	A	2273	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6172 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.

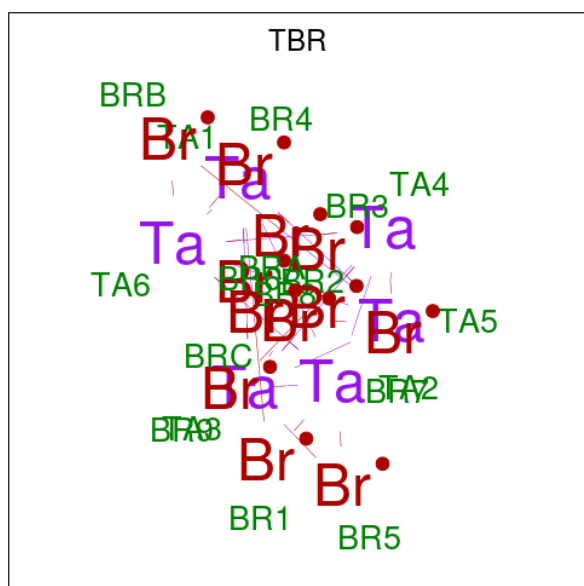
- Molecule 1 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1248	792	219	232	5			
1	C	185	Total	C	N	O	S	0	0	0
			1248	792	219	232	5			

- Molecule 2 is a protein called PROTEIN CAF40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			1820	1174	306	330	10			
2	D	261	Total	C	N	O	S	0	0	0
			1802	1155	309	327	11			

- Molecule 3 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).

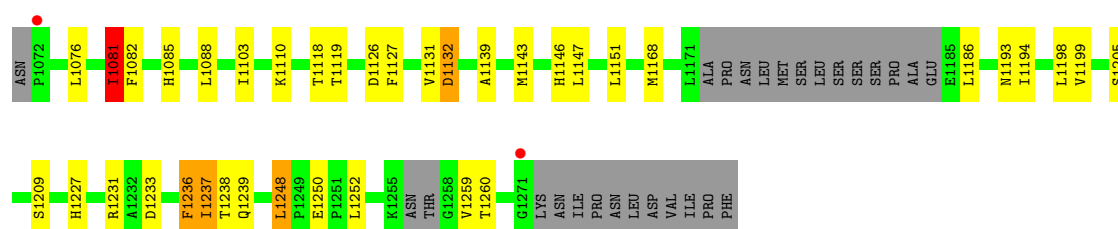


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 18	Br 12	Ta 6	0	0
3	A	1	Total 18	Br 12	Ta 6	0	0
3	B	1	Total 18	Br 12	Ta 6	0	0

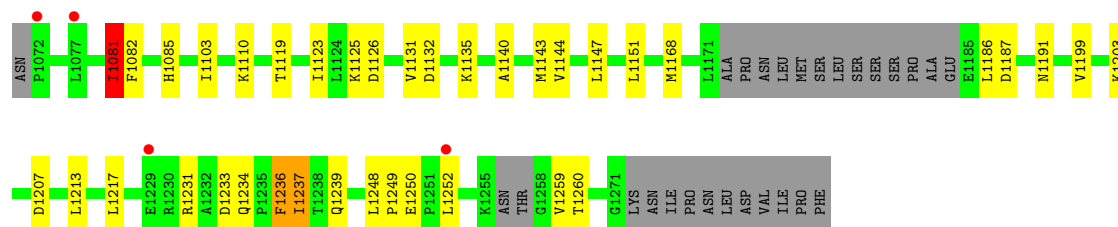
3 Residue-property plots [i](#)

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.

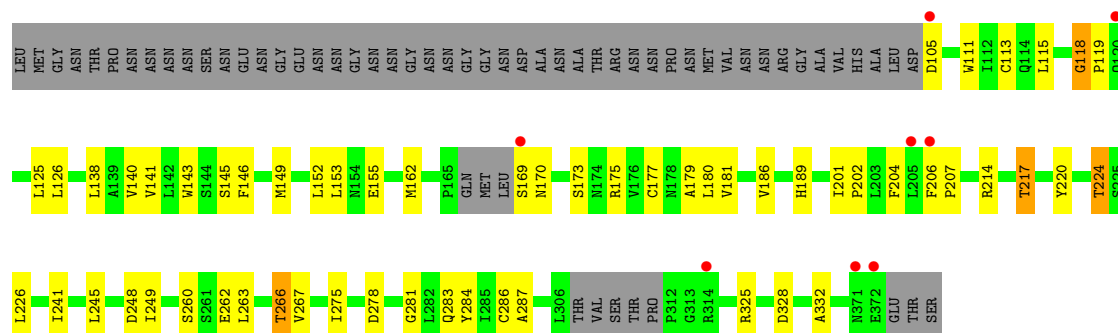
• Molecule 1: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1



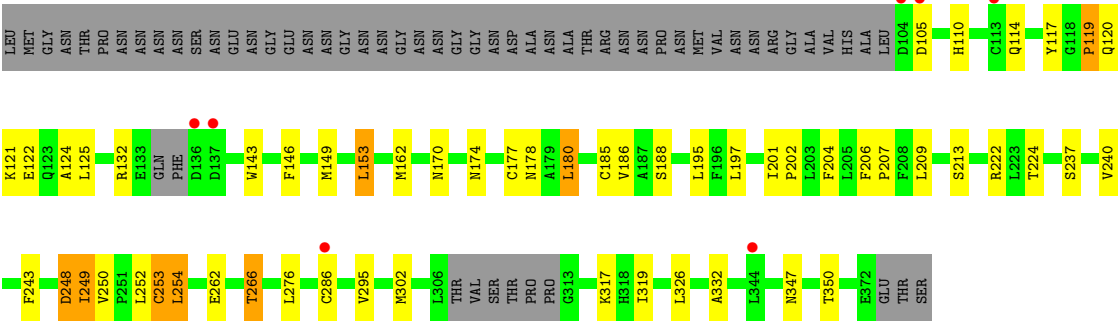
• Molecule 1: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1



• Molecule 2: PROTEIN CAF40



• Molecule 2: PROTEIN CAF40



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.34Å 188.34Å 126.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 3.81 48.29 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.29-3.81) 99.8 (48.29-3.81)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.276 , 0.295 0.295 , 0.307	Depositor DCC
R_{free} test set	1143 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	148.8	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 122.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6172	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

Bond lengths and bond angles in the following residue types are not validated in this section: TBR

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	0.36	0/1261	0.86	3/1722 (0.2%)
1	C	0.36	0/1261	0.86	3/1722 (0.2%)
2	B	0.33	0/1851	0.81	7/2542 (0.3%)
2	D	0.33	0/1831	0.82	2/2512 (0.1%)
All	All	0.34	0/6204	0.84	15/8498 (0.2%)

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
2	D	0	2
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	248	ASP	N-CA-C	6.58	120.59	107.62
2	B	118	GLY	CA-C-N	6.43	125.93	119.24
2	B	118	GLY	C-N-CA	6.43	125.93	119.24
1	C	1085	HIS	CA-C-N	6.24	125.46	118.97
1	C	1085	HIS	C-N-CA	6.24	125.46	118.97
1	A	1085	HIS	CA-C-N	6.02	125.50	119.24
1	A	1085	HIS	C-N-CA	6.02	125.50	119.24
2	B	105	ASP	CA-C-N	-5.73	112.68	119.84
2	B	105	ASP	C-N-CA	-5.73	112.68	119.84
2	B	260	SER	CB-CA-C	-5.65	110.07	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1248	LEU	N-CA-C	5.39	121.72	109.81
1	A	1248	LEU	N-CA-C	5.21	121.32	109.81
2	B	189	HIS	CA-C-N	5.11	125.14	119.32
2	B	189	HIS	C-N-CA	5.11	125.14	119.32
2	D	105	ASP	N-CA-C	5.04	119.11	112.35

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1248	LEU	Peptide
2	D	119	PRO	Peptide
2	D	248	ASP	Peptide

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	1248	0	1163	25	0
1	C	1248	0	1164	20	0
2	B	1820	0	1648	29	0
2	D	1802	0	1613	31	0
3	A	36	0	0	6	0
3	B	18	0	0	1	0
All	All	6172	0	5588	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (97) 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:1238:THR:HB	3:A:2273:TBR:BR7	2.02	1.15
2:B:278:ASP:OD1	3:B:1373:TBR:BRB	2.59	0.76
2:D:249:ILE:HG23	2:D:250:VAL:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:ILE:HG23	1:A:1082:PHE:H	1.55	0.71
1:A:1238:THR:CB	3:A:2273:TBR:BR7	2.88	0.71
1:C:1081:ILE:HG23	1:C:1082:PHE:H	1.57	0.69
1:A:1250:GLU:O	1:A:1252:LEU:N	2.26	0.68
1:C:1250:GLU:O	1:C:1252:LEU:N	2.25	0.67
2:D:121:LYS:O	2:D:124:ALA:N	2.27	0.67
2:D:149:MET:HE1	2:D:186:VAL:HG21	1.77	0.66
2:D:213:SER:O	2:D:222:ARG:NH2	2.29	0.66
2:D:250:VAL:HA	2:D:253:CYS:HB2	1.77	0.66
2:D:122:GLU:HA	2:D:125:LEU:HB2	1.77	0.65
1:A:1238:THR:O	3:A:2273:TBR:BR8	2.70	0.64
1:C:1203:LYS:NZ	1:C:1207:ASP:OD2	2.30	0.62
2:B:325:ARG:NH1	2:B:328:ASP:OD2	2.35	0.59
1:A:1131:VAL:HG22	1:A:1132:ASP:H	1.68	0.58
2:D:209:LEU:HB3	2:D:252:LEU:HD21	1.86	0.58
1:A:1146:HIS:ND1	3:A:2272:TBR:BR2	2.93	0.56
1:C:1131:VAL:HG22	1:C:1132:ASP:H	1.70	0.55
2:D:185:CYS:O	2:D:188:SER:OG	2.22	0.54
2:D:347:ASN:OD1	2:D:350:THR:OG1	2.20	0.54
2:B:245:LEU:HD22	2:B:284:TYR:HD2	1.73	0.54
2:B:262:GLU:O	2:B:266:THR:OG1	2.25	0.53
2:B:220:TYR:O	2:B:224:THR:OG1	2.26	0.53
1:A:1238:THR:O	3:A:2273:TBR:BRB	2.81	0.53
1:C:1147:LEU:HD21	2:D:204:PHE:HZ	1.73	0.53
2:B:149:MET:HE1	2:B:186:VAL:HG21	1.91	0.52
1:C:1233:ASP:N	1:C:1233:ASP:OD1	2.41	0.51
2:B:143:TRP:HE3	2:B:149:MET:HE3	1.76	0.51
2:B:155:GLU:OE1	2:B:175:ARG:NE	2.43	0.51
1:A:1239:GLN:O	3:A:2273:TBR:BRB	2.83	0.51
2:B:245:LEU:HD11	2:B:281:GLY:HA2	1.92	0.51
1:A:1237:ILE:HG22	1:A:1239:GLN:N	2.26	0.51
1:A:1147:LEU:HD21	2:B:204:PHE:HZ	1.76	0.50
1:C:1236:PHE:CG	1:C:1237:ILE:HG12	2.47	0.50
1:C:1187:ASP:O	1:C:1191:ASN:ND2	2.31	0.50
2:D:170:ASN:OD1	2:D:170:ASN:N	2.46	0.49
1:A:1205:SER:O	1:A:1209:SER:OG	2.23	0.49
2:D:122:GLU:HA	2:D:125:LEU:HD12	1.95	0.49
2:D:174:ASN:O	2:D:178:ASN:ND2	2.46	0.49
1:C:1237:ILE:HG22	1:C:1239:GLN:N	2.27	0.48
2:B:115:LEU:HD21	2:B:152:LEU:HD21	1.96	0.48
1:A:1236:PHE:CG	1:A:1237:ILE:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:CYS:HA	2:B:180:LEU:HD12	1.97	0.46
2:B:226:LEU:HB3	2:B:267:VAL:HG11	1.96	0.46
2:D:262:GLU:O	2:D:266:THR:OG1	2.33	0.46
1:C:1132:ASP:O	1:C:1135:LYS:N	2.49	0.46
2:D:177:CYS:HA	2:D:180:LEU:HB2	1.97	0.46
2:B:141:VAL:O	2:B:145:SER:OG	2.27	0.46
2:B:286:CYS:SG	2:B:332:ALA:HB2	2.55	0.46
2:D:201:ILE:N	2:D:202:PRO:HD2	2.30	0.46
1:A:1233:ASP:OD1	1:A:1233:ASP:N	2.41	0.45
2:D:149:MET:O	2:D:153:LEU:HB2	2.16	0.45
1:C:1123:ILE:HD13	1:C:1140:ALA:HA	1.98	0.45
1:A:1119:THR:HG22	1:A:1143:MET:HE2	1.99	0.45
1:C:1126:ASP:HB3	2:D:146:PHE:CE1	2.52	0.45
1:A:1147:LEU:HD21	2:B:204:PHE:CZ	2.51	0.45
2:B:170:ASN:O	2:B:173:SER:N	2.37	0.45
1:A:1194:ILE:HG12	1:A:1198:LEU:HD13	1.99	0.44
2:B:125:LEU:HD21	2:B:179:ALA:HB2	1.99	0.44
2:B:169:SER:C	2:B:217:THR:HG21	2.43	0.44
1:C:1125:LYS:NZ	2:D:143:TRP:O	2.42	0.44
2:D:110:HIS:O	2:D:114:GLN:HG2	2.17	0.44
1:C:1259:VAL:HG22	1:C:1260:THR:H	1.83	0.44
2:D:132:ARG:HG3	2:D:185:CYS:HB2	1.99	0.44
2:D:286:CYS:SG	2:D:332:ALA:HB2	2.57	0.44
2:B:143:TRP:CE3	2:B:149:MET:HE3	2.53	0.44
1:A:1126:ASP:HB3	2:B:146:PHE:CE2	2.53	0.43
2:D:302:MET:HE3	2:D:319:ILE:HD11	2.00	0.43
1:A:1088:LEU:HD12	1:A:1088:LEU:HA	1.82	0.43
1:A:1252:LEU:O	2:B:146:PHE:N	2.41	0.43
2:B:206:PHE:CZ	2:B:249:ILE:HB	2.53	0.43
1:A:1076:LEU:HB3	1:A:1193:ASN:ND2	2.32	0.43
1:C:1147:LEU:HD21	2:D:204:PHE:CZ	2.54	0.43
1:C:1231:ARG:HB2	1:C:1234:GLN:HG3	2.01	0.43
2:D:162:MET:N	2:D:162:MET:SD	2.92	0.42
2:D:237:SER:HB3	2:D:240:VAL:HG23	2.01	0.42
2:D:276:LEU:HD22	2:D:326:LEU:HD21	2.01	0.42
2:B:206:PHE:N	2:B:207:PRO:HD2	2.34	0.42
1:C:1213:LEU:O	1:C:1217:LEU:N	2.52	0.42
1:A:1259:VAL:HG22	1:A:1260:THR:H	1.84	0.42
2:B:283:GLN:O	2:B:287:ALA:HB2	2.20	0.42
1:A:1127:PHE:HD1	1:A:1127:PHE:HA	1.79	0.41
2:D:254:LEU:HD21	2:D:295:VAL:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:HIS:O	1:A:1227:HIS:ND1	2.54	0.41
2:D:197:LEU:HD11	2:D:243:PHE:CG	2.55	0.41
2:B:118:GLY:HA2	2:B:119:PRO:HD3	1.79	0.41
2:D:206:PHE:N	2:D:207:PRO:HD2	2.35	0.41
1:A:1127:PHE:HE2	1:A:1139:ALA:HB3	1.85	0.41
1:C:1103:ILE:H	1:C:1103:ILE:HG13	1.73	0.41
1:C:1119:THR:HG22	1:C:1143:MET:HG2	2.02	0.41
2:D:143:TRP:CZ2	2:D:195:LEU:HB3	2.56	0.41
2:B:241:ILE:HD12	2:B:275:ILE:HA	2.03	0.40
1:C:1144:VAL:HG11	1:C:1213:LEU:HD22	2.02	0.40
2:B:111:TRP:CE3	2:B:111:TRP:HA	2.57	0.40
2:B:201:ILE:N	2:B:202:PRO:HD2	2.36	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	179/212 (84%)	163 (91%)	14 (8%)	2 (1%)	11	41
1	C	179/212 (84%)	165 (92%)	11 (6%)	3 (2%)	7	34
2	B	254/320 (79%)	240 (94%)	14 (6%)	0	100	100
2	D	255/320 (80%)	242 (95%)	10 (4%)	3 (1%)	10	40
All	All	867/1064 (82%)	810 (93%)	49 (6%)	8 (1%)	14	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	120	GLN
2	D	249	ILE
1	A	1081	ILE

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Mol	Chain	Res	Type
1	A	1237	ILE
1	C	1081	ILE
1	C	1237	ILE
2	D	119	PRO
1	C	1249	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	110/187 (59%)	99 (90%)	11 (10%)	7	28
1	C	110/187 (59%)	103 (94%)	7 (6%)	16	42
2	B	166/289 (57%)	153 (92%)	13 (8%)	11	36
2	D	162/289 (56%)	154 (95%)	8 (5%)	22	47
All	All	548/952 (58%)	509 (93%)	39 (7%)	13	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1081	ILE
1	A	1103	ILE
1	A	1110	LYS
1	A	1118	THR
1	A	1132	ASP
1	A	1151	LEU
1	A	1168	MET
1	A	1186	LEU
1	A	1199	VAL
1	A	1231	ARG
1	A	1236	PHE
2	B	113	CYS
2	B	126	LEU
2	B	138	LEU
2	B	140	VAL
2	B	153	LEU

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Mol	Chain	Res	Type
2	B	162	MET
2	B	181	VAL
2	B	214	ARG
2	B	217	THR
2	B	224	THR
2	B	248	ASP
2	B	263	LEU
2	B	266	THR
1	C	1081	ILE
1	C	1110	LYS
1	C	1151	LEU
1	C	1168	MET
1	C	1186	LEU
1	C	1199	VAL
1	C	1236	PHE
2	D	117	TYR
2	D	153	LEU
2	D	180	LEU
2	D	224	THR
2	D	253	CYS
2	D	254	LEU
2	D	266	THR
2	D	317	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1093	GLN
2	D	114	GLN
2	D	174	ASN
2	D	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TBR	A	2272	-	0,36,36	-	-	-		
3	TBR	B	1373	-	0,36,36	-	-	-		
3	TBR	A	2273	-	0,36,36	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2272	TBR	1	0
3	B	1373	TBR	1	0
3	A	2273	TBR	5	0

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	185/212 (87%)	-0.06	2 (1%) 78 56	32, 87, 163, 241	0
1	C	185/212 (87%)	0.10	4 (2%) 62 44	35, 93, 166, 261	0
2	B	260/320 (81%)	0.03	8 (3%) 51 35	37, 83, 167, 239	0
2	D	261/320 (81%)	-0.07	7 (2%) 56 38	43, 85, 156, 198	0
All	All	891/1064 (83%)	-0.00	21 (2%) 59 41	32, 87, 165, 261	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	169	SER	5.5
2	D	104	ASP	4.3
1	C	1072	PRO	4.1
2	B	105	ASP	4.0
2	D	105	ASP	3.8
2	B	206	PHE	3.8
1	A	1271	GLY	3.6
1	C	1077	LEU	3.5
2	B	205	LEU	3.4
1	C	1252	LEU	3.2
2	B	372	GLU	2.9
2	D	344	LEU	2.8
2	D	286	CYS	2.7
2	B	371	ASN	2.7
2	D	137	ASP	2.6
2	D	136	ASP	2.4
2	D	113	CYS	2.3
2	B	314	ARG	2.3
2	B	120	GLN	2.1
1	A	1072	PRO	2.0
1	C	1229	GLU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TBR	A	2273	18/18	0.74	0.21	121,162,194,201	18
3	TBR	B	1373	18/18	0.76	0.20	104,146,178,185	18
3	TBR	A	2272	18/18	0.86	0.19	147,189,220,228	18

6.5 Other polymers [i](#)

There are no such residues in this entry.