



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 25, 2017 – 11:03 AM EST

PDB ID : 6F9N
Title : CRYSTAL STRUCTURE OF THE HUMAN CPSF160-WDR33 COMPLEX
Authors : Clerici, M.; Jinek, M.
Deposited on : 2017-12-14
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

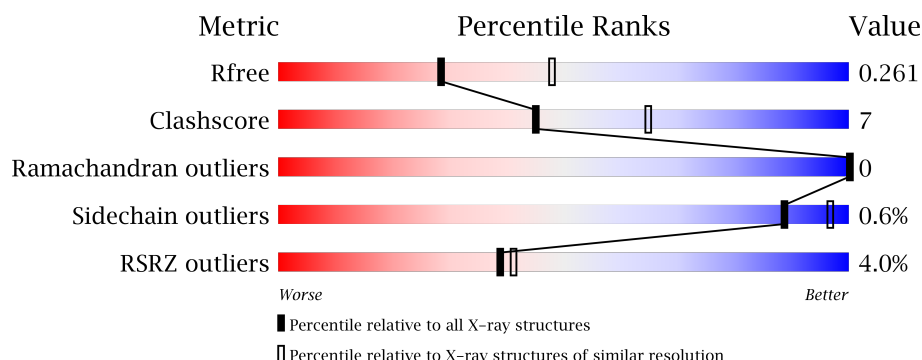
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1443	<div> <div>3%</div> <div>66%</div> <div>15%</div> <div>18%</div> </div>
2	B	379	<div> <div>4%</div> <div>73%</div> <div>21%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12264 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 Cleavage and polyadenylation specificity factor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1180	Total	C	N	O	S	0	0	0
			9290	5970	1586	1679	55			

- Molecule 2 is a protein called pre-mRNA 3' end processing protein WDR33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	357	Total	C	N	O	S	0	0	0
			2872	1816	522	516	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	32	SER	-	expression tag	UNP Q9C0J8
B	33	ASN	-	expression tag	UNP Q9C0J8
B	34	ALA	-	expression tag	UNP Q9C0J8

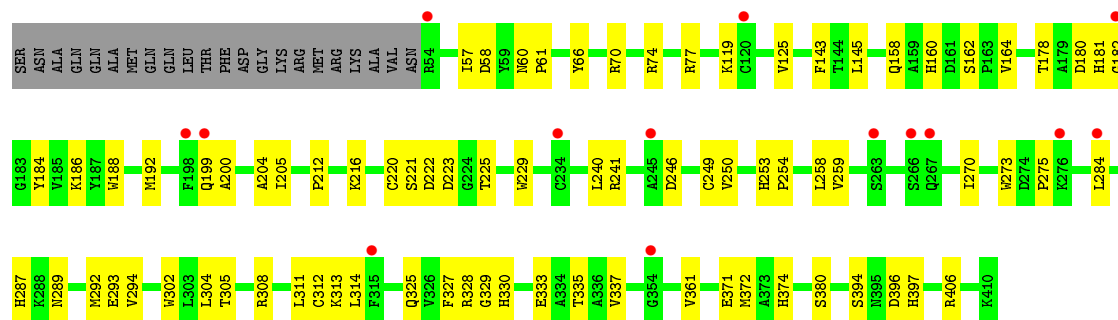
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	33	Total	O	0	0
			33	33		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A: ■ 66% ■ 15% ■ 18%

- Molecule 2: pre-mRNA 3' end processing protein WDR33



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.91Å 77.40Å 104.02Å 87.56° 76.41° 67.00°	Depositor
Resolution (Å)	47.31 – 2.50 47.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.31-2.50) 98.1 (47.31-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.228 , 0.263 0.224 , 0.261	Depositor DCC
R_{free} test set	3269 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12264	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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	0.25	0/9502	0.46	1/12903 (0.0%)
2	B	0.25	0/2955	0.44	0/4005
All	All	0.25	0/12457	0.46	1/16908 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ALA	N-CA-CB	-6.70	100.72	110.10

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	9290	0	9287	133	0
2	B	2872	0	2780	48	0
3	A	69	0	0	1	0
3	B	33	0	0	1	0
All	All	12264	0	12067	180	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 7.

All (180) 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:182:GLY:H	2:B:204:ALA:HA	1.42	0.83
1:A:1184:SER:HB3	1:A:1193:TRP:HZ3	1.47	0.77
1:A:948:PRO:HA	1:A:971:PRO:HB3	1.70	0.73
1:A:1109:ARG:HG3	1:A:1180:GLY:HA3	1.69	0.72
2:B:304:LEU:HD22	2:B:337:VAL:HG11	1.75	0.67
1:A:100:ASP:O	1:A:139:PRO:HG3	1.94	0.66
1:A:1051:THR:HA	1:A:1133:VAL:HG13	1.77	0.66
1:A:812:PRO:HB2	1:A:844:PRO:HB2	1.77	0.65
1:A:218:LEU:HD13	1:A:278:VAL:HG11	1.78	0.65
2:B:178:THR:HG1	2:B:188:TRP:HE1	1.44	0.64
1:A:101:ALA:HB3	1:A:124:GLU:HG3	1.80	0.64
1:A:67:GLU:HA	1:A:958:ARG:HA	1.79	0.64
2:B:164:VAL:HA	2:B:180:ASP:HA	1.81	0.63
1:A:351:THR:HB	1:A:355:ARG:HA	1.80	0.62
1:A:696:ILE:HG22	1:A:697:THR:HG23	1.80	0.62
1:A:789:ARG:NH1	1:A:795:GLU:OE2	2.31	0.62
1:A:1280:VAL:HB	1:A:1300:ALA:HB3	1.80	0.62
1:A:1262:VAL:HB	1:A:1334:HIS:HB2	1.82	0.61
1:A:1425:THR:HG22	1:A:1427:ASP:H	1.66	0.61
1:A:937:ILE:HD11	1:A:987:PHE:HB3	1.82	0.60
1:A:1365:ALA:HB1	1:A:1418:LEU:HD11	1.84	0.60
1:A:25:ASN:ND2	1:A:89:ALA:O	2.33	0.60
2:B:259:VAL:HG23	2:B:275:PRO:HG3	1.84	0.59
1:A:903:GLU:HG2	1:A:948:PRO:HB3	1.85	0.59
1:A:157:THR:HG22	1:A:158:ARG:HE	1.67	0.58
1:A:483:PRO:HG3	1:A:499:GLU:HB2	1.84	0.58
2:B:145:LEU:HD11	2:B:192:MET:HG3	1.85	0.58
1:A:1177:HIS:O	1:A:1217:SER:OG	2.17	0.57
2:B:222:ASP:HA	2:B:246:ASP:HA	1.85	0.57
2:B:308:ARG:HA	2:B:333:GLU:HB3	1.85	0.57
1:A:1095:GLN:OE1	1:A:1138:ARG:NH1	2.38	0.57
2:B:312:CYS:HB2	2:B:327:PHE:HB2	1.87	0.56
1:A:251:VAL:HG12	1:A:253:PRO:HD3	1.87	0.56
1:A:163:PRO:HB2	1:A:186:LEU:HB2	1.87	0.56
2:B:325:GLN:NE2	2:B:361:VAL:O	2.35	0.56
1:A:1141:ILE:HB	1:A:1164:TYR:HB3	1.88	0.56
1:A:374:MET:HE3	1:A:382:LEU:HD11	1.88	0.56
1:A:245:LEU:HD23	1:A:252:HIS:HB3	1.88	0.55
2:B:270:ILE:HB	2:B:284:LEU:HB3	1.87	0.55
1:A:1050:MET:HG3	1:A:1053:GLU:HB2	1.89	0.55
1:A:1435:GLU:OE2	1:A:1438:ARG:NH2	2.40	0.55
1:A:283:VAL:HG22	1:A:323:ASP:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:OG1	1:A:36:SER:N	2.39	0.54
1:A:113:HIS:HB3	1:A:893:LYS:HD2	1.90	0.54
2:B:394:SER:OG	2:B:396:ASP:OD1	2.26	0.53
1:A:1258:VAL:HG23	1:A:1271:VAL:HG22	1.91	0.53
1:A:990:PHE:CE1	1:A:996:LEU:HB2	2.43	0.53
1:A:626:ILE:HD11	1:A:658:ILE:HD13	1.91	0.53
1:A:991:ASN:HD21	1:A:995:GLU:HB2	1.72	0.53
2:B:158:GLN:NE2	2:B:160:HIS:O	2.41	0.53
1:A:932:ARG:HG3	1:A:975:PHE:HB3	1.91	0.53
1:A:302:SER:HB2	1:A:1065:ARG:HB2	1.91	0.53
1:A:704:LEU:HD12	1:A:858:GLN:HG3	1.91	0.53
2:B:293:GLU:OE1	2:B:337:VAL:N	2.39	0.52
1:A:796:ILE:HB	1:A:806:PHE:HB3	1.92	0.52
1:A:617:TYR:OH	1:A:678:ARG:O	2.27	0.52
1:A:1139:ILE:HG13	1:A:1168:GLN:HG3	1.91	0.52
1:A:336:VAL:HG22	1:A:346:VAL:HG22	1.92	0.52
2:B:258:LEU:HA	2:B:275:PRO:HD3	1.92	0.52
1:A:587:GLN:HG2	1:A:595:LEU:HD22	1.92	0.51
2:B:160:HIS:CE1	2:B:186:LYS:HG3	2.46	0.51
1:A:472:ILE:HD13	1:A:515:LEU:HD21	1.92	0.51
1:A:1353:GLU:O	1:A:1357:ARG:HG2	2.10	0.51
2:B:221:SER:OG	2:B:223:ASP:OD1	2.22	0.51
1:A:4:VAL:HG12	1:A:1399:LEU:HB2	1.92	0.51
2:B:302:TRP:HB3	2:B:314:LEU:HD11	1.91	0.51
2:B:249:CYS:HB2	2:B:294:VAL:HG12	1.93	0.51
1:A:1263:ASP:OD1	1:A:1264:ASN:N	2.42	0.51
2:B:292:MET:HG2	2:B:335:THR:HA	1.94	0.50
1:A:29:ASN:ND2	3:A:1508:HOH:O	2.42	0.50
1:A:299:ALA:HB1	1:A:304:THR:HG21	1.94	0.50
1:A:4:VAL:HG12	1:A:1399:LEU:HD12	1.94	0.50
1:A:108:TYR:OH	1:A:113:HIS:ND1	2.38	0.49
1:A:1234:LEU:HD23	1:A:1245:LEU:HA	1.94	0.49
1:A:856:SER:HB3	1:A:957:GLY:HA2	1.94	0.49
1:A:344:ILE:HD11	1:A:384:LEU:HD11	1.93	0.49
1:A:653:ASP:O	1:A:702:ARG:NH1	2.46	0.49
1:A:97:SER:HB3	1:A:139:PRO:HB2	1.93	0.49
2:B:119:LYS:HB3	2:B:397:HIS:HB3	1.93	0.49
1:A:848:GLU:HB3	1:A:866:HIS:HB3	1.93	0.49
1:A:969:ASP:OD2	1:A:997:ARG:NH1	2.46	0.49
1:A:1363:GLN:HG3	1:A:1403:LEU:HD23	1.95	0.49
2:B:184:TYR:CE2	2:B:199:GLN:HG2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:LYS:NZ	3:B:502:HOH:O	2.35	0.48
1:A:648:GLN:HB2	1:A:659:MET:HG2	1.94	0.48
1:A:130:ASP:OD1	1:A:158:ARG:NH2	2.47	0.48
2:B:311:LEU:HD22	2:B:328:ARG:HG2	1.96	0.48
1:A:586:LEU:HD23	1:A:594:GLU:HA	1.95	0.48
1:A:673:ASP:OD1	1:A:677:GLY:N	2.46	0.48
1:A:705:SER:OG	1:A:706:GLY:N	2.47	0.48
1:A:934:PHE:HB3	1:A:977:PRO:HG3	1.96	0.47
1:A:583:THR:HG22	1:A:602:THR:HA	1.95	0.47
1:A:1183:VAL:HG11	1:A:1222:ILE:HD13	1.97	0.47
1:A:903:GLU:OE2	1:A:992:ARG:NH2	2.43	0.47
1:A:111:GLY:O	1:A:891:ARG:NH1	2.46	0.47
1:A:140:ARG:HH11	1:A:153:LEU:HD23	1.79	0.47
1:A:371:THR:HG22	1:A:384:LEU:HB3	1.97	0.47
1:A:1261:MET:HG2	1:A:1270:LEU:HB2	1.96	0.47
1:A:1283:TYR:CZ	1:A:1285:PRO:HG3	2.50	0.47
1:A:99:LYS:HA	1:A:99:LYS:HD2	1.66	0.47
2:B:240:LEU:HB3	2:B:273:TRP:CE3	2.49	0.47
1:A:869:GLN:HB3	1:A:902:ARG:HG2	1.95	0.47
1:A:988:LEU:HA	1:A:997:ARG:O	2.15	0.47
2:B:374:HIS:CE1	2:B:394:SER:HG	2.33	0.47
1:A:8:ALA:HB1	1:A:1011:TRP:HZ2	1.79	0.46
2:B:180:ASP:N	2:B:180:ASP:OD1	2.49	0.46
1:A:629:LEU:HB3	1:A:634:GLN:HA	1.96	0.46
1:A:793:THR:HG22	1:A:809:LYS:HA	1.97	0.46
1:A:861:PRO:HG2	1:A:876:ALA:HB3	1.98	0.46
1:A:937:ILE:HD13	1:A:952:TRP:HZ3	1.80	0.46
1:A:867:VAL:HG12	1:A:868:ASP:H	1.80	0.46
2:B:287:HIS:CE1	2:B:313:LYS:HG3	2.51	0.46
1:A:1018:LEU:HD12	1:A:1022:ALA:HB2	1.97	0.45
1:A:1137:GLY:HA3	1:A:1172:VAL:HG23	1.99	0.45
1:A:1425:THR:HB	1:A:1428:ILE:HG13	1.97	0.45
1:A:991:ASN:ND2	1:A:995:GLU:HB2	2.31	0.45
2:B:57:ILE:HG22	2:B:406:ARG:HH22	1.82	0.45
1:A:612:ILE:HG22	1:A:670:LEU:HD22	1.99	0.45
1:A:515:LEU:HG	1:A:1013:VAL:HG12	1.99	0.44
1:A:1311:PHE:CD1	1:A:1338:PHE:HB3	2.52	0.44
1:A:988:LEU:HD13	1:A:996:LEU:HD11	1.99	0.44
1:A:102:LYS:HG3	1:A:124:GLU:OE1	2.18	0.44
1:A:1216:ILE:HG22	1:A:1260:PHE:HE2	1.81	0.44
1:A:14:LEU:O	1:A:372:THR:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:THR:HG22	2:B:241:ARG:HG2	2.00	0.44
1:A:1193:TRP:CD1	1:A:1202:GLY:HA2	2.53	0.44
2:B:143:PHE:CZ	2:B:178:THR:HG21	2.52	0.44
1:A:1128:MET:HB2	2:B:61:PRO:HB3	1.99	0.44
1:A:936:ASP:OD2	1:A:985:ARG:NH1	2.51	0.44
1:A:398:GLU:HG2	1:A:398:GLU:H	1.64	0.43
2:B:200:ALA:HB3	2:B:205:ILE:HD11	2.00	0.43
1:A:499:GLU:OE2	1:A:516:GLN:NE2	2.49	0.43
1:A:806:PHE:CE1	1:A:820:ASP:HB2	2.54	0.43
1:A:1190:ILE:HG13	1:A:1208:THR:HG21	2.00	0.43
1:A:973:ASP:OD1	1:A:973:ASP:N	2.51	0.43
1:A:1190:ILE:O	1:A:1205:PHE:HA	2.18	0.43
1:A:1435:GLU:O	1:A:1439:VAL:HG23	2.19	0.43
2:B:289:ASN:HB3	2:B:308:ARG:HB2	1.99	0.43
2:B:204:ALA:O	2:B:222:ASP:N	2.48	0.43
1:A:216:THR:HA	1:A:243:ILE:O	2.19	0.43
1:A:1050:MET:HB2	1:A:1054:GLU:O	2.19	0.42
1:A:495:GLU:HG3	1:A:1317:ARG:CZ	2.49	0.42
1:A:621:VAL:HG22	1:A:626:ILE:HG23	2.01	0.42
1:A:651:VAL:HG22	1:A:656:VAL:HG13	2.00	0.42
1:A:318:VAL:HG21	1:A:362:PHE:CD1	2.54	0.42
2:B:125:VAL:HG22	2:B:380:SER:HB3	2.01	0.42
2:B:220:CYS:HB3	2:B:250:VAL:HB	2.02	0.42
2:B:240:LEU:HD13	2:B:273:TRP:CG	2.55	0.42
2:B:371:GLU:HB3	2:B:372:MET:SD	2.59	0.42
1:A:577:LEU:O	1:A:583:THR:OG1	2.24	0.42
2:B:74:ARG:NH2	2:B:77:ARG:HH21	2.18	0.42
1:A:629:LEU:CB	1:A:634:GLN:HA	2.50	0.42
2:B:162:SER:OG	2:B:181:HIS:O	2.22	0.42
2:B:304:LEU:HD23	2:B:305:THR:N	2.34	0.42
1:A:101:ALA:HB1	1:A:123:PHE:HB2	2.01	0.42
2:B:329:GLY:O	2:B:330:HIS:ND1	2.53	0.42
1:A:372:THR:HG22	1:A:386:SER:HA	2.02	0.41
1:A:587:GLN:O	1:A:592:ILE:HA	2.20	0.41
1:A:953:LEU:HA	1:A:962:ARG:O	2.20	0.41
2:B:253:HIS:CG	2:B:254:PRO:HD2	2.54	0.41
2:B:66:TYR:O	2:B:70:ARG:HG3	2.20	0.41
1:A:354:MET:N	1:A:354:MET:SD	2.93	0.41
1:A:66:LEU:HD11	1:A:393:LEU:HD22	2.01	0.41
1:A:786:LEU:HD22	1:A:849:VAL:HG21	2.01	0.41
1:A:952:TRP:HE1	1:A:966:MET:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1379:ARG:O	1:A:1383:MET:HG2	2.20	0.41
1:A:670:LEU:HG	1:A:680:HIS:HB3	2.02	0.41
1:A:215:PRO:HG2	1:A:245:LEU:HB2	2.02	0.41
2:B:212:PRO:HB3	2:B:254:PRO:O	2.20	0.41
1:A:1276:ARG:HB3	1:A:1306:ALA:N	2.36	0.41
1:A:1407:TYR:HD1	1:A:1418:LEU:HD23	1.85	0.41
2:B:270:ILE:CD1	2:B:305:THR:HG21	2.50	0.41
1:A:1407:TYR:CE2	1:A:1415:ARG:HD2	2.56	0.41
1:A:600:PHE:CE1	1:A:629:LEU:HD11	2.56	0.41
1:A:687:PRO:HB3	1:A:802:TRP:CE2	2.56	0.41
1:A:512:LEU:HG	1:A:1018:LEU:HD11	2.02	0.40
1:A:38:LEU:HB2	1:A:74:PHE:HE2	1.86	0.40
2:B:58:ASP:OD1	2:B:60:ASN:ND2	2.40	0.40
1:A:123:PHE:CZ	1:A:160:VAL:HG11	2.56	0.40
1:A:969:ASP:OD1	1:A:970:GLY:N	2.51	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	1152/1443 (80%)	1096 (95%)	56 (5%)	0	100	100
2	B	355/379 (94%)	329 (93%)	26 (7%)	0	100	100
All	All	1507/1822 (83%)	1425 (95%)	82 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	1018/1235 (82%)	1011 (99%)	7 (1%)	87	96
2	B	309/327 (94%)	308 (100%)	1 (0%)	94	98
All	All	1327/1562 (85%)	1319 (99%)	8 (1%)	89	97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	TRP
1	A	629	LEU
1	A	689	LEU
1	A	691	HIS
1	A	990	PHE
1	A	1160	PHE
1	A	1299	ARG
2	B	229	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1180/1443 (81%)	0.30	47 (3%) 39 41	33, 65, 108, 174	0
2	B	357/379 (94%)	0.31	14 (3%) 40 42	38, 71, 110, 139	0
All	All	1537/1822 (84%)	0.30	61 (3%) 39 41	33, 66, 108, 174	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	690	HIS	4.5
1	A	689	LEU	4.4
1	A	1051	THR	4.0
1	A	185	PHE	3.9
1	A	1155	LEU	3.8
1	A	616	ARG	3.6
1	A	1055	LYS	3.4
1	A	1386	VAL	3.2
2	B	54	ARG	3.1
2	B	267	GLN	3.0
1	A	1331	GLU	3.0
1	A	1287	ALA	2.9
1	A	1289	GLU	2.8
2	B	245	ALA	2.8
1	A	677	GLY	2.7
1	A	182	ARG	2.7
2	B	266	SER	2.6
1	A	99	LYS	2.6
1	A	805	VAL	2.6
1	A	1291	PHE	2.6
2	B	315	PHE	2.6
1	A	87	ALA	2.6
1	A	293	VAL	2.6
1	A	671	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1219	LYS	2.5
1	A	1057	PHE	2.5
2	B	198	PHE	2.5
2	B	120	CYS	2.5
1	A	292	SER	2.5
1	A	89	ALA	2.5
1	A	247	ILE	2.4
2	B	263	SER	2.4
1	A	696	ILE	2.3
1	A	183	SER	2.3
1	A	709	THR	2.3
1	A	355	ARG	2.3
1	A	162	LEU	2.3
1	A	1339	ALA	2.3
1	A	88	GLY	2.3
1	A	626	ILE	2.2
2	B	234	CYS	2.2
1	A	1428	ILE	2.2
1	A	11	PRO	2.2
1	A	353	GLY	2.2
1	A	959	GLY	2.2
2	B	182	GLY	2.2
1	A	313	ARG	2.2
2	B	354	GLY	2.1
1	A	245	LEU	2.1
1	A	1114	VAL	2.1
1	A	200	LEU	2.1
1	A	1216	ILE	2.1
1	A	1344	GLY	2.1
1	A	475	CYS	2.1
1	A	541	PRO	2.1
1	A	312	LEU	2.1
2	B	199	GLN	2.1
2	B	284	LEU	2.0
2	B	276	LYS	2.0
1	A	350	ILE	2.0
1	A	1112	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.