



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:27 PM UTC

PDB ID : 6F9N / pdb_00006f9n
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

<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

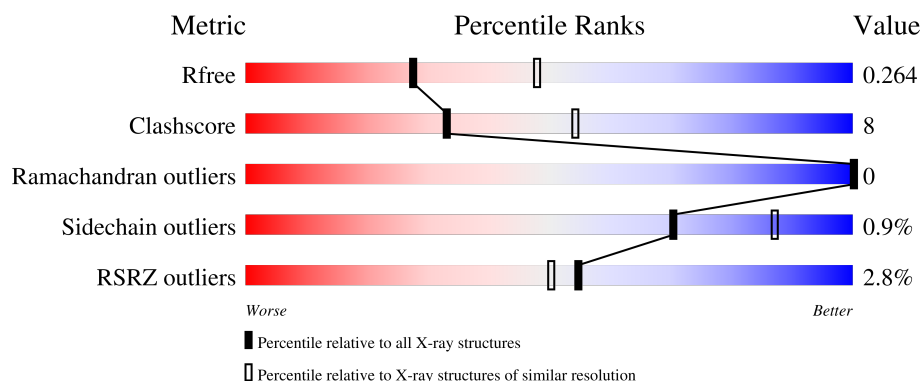
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

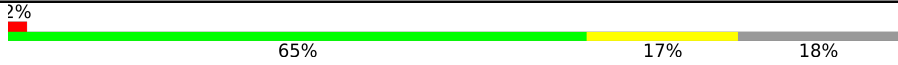
The reported resolution of this entry is 2.50 Å.

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	1443	
2	B	379	

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:

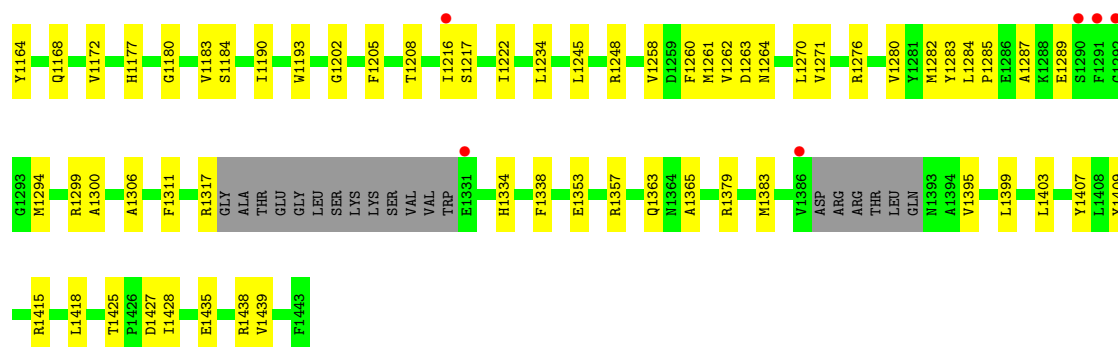
Chain	Residue	Modelled	Actual	Comment	Reference
B	32	SER	-	expression tag	UNP Q9C0J8
B	33	ASN	-	expression tag	UNP Q9C0J8
B	34	ALA	-	expression tag	UNP Q9C0J8

- Molecule 3 is water.

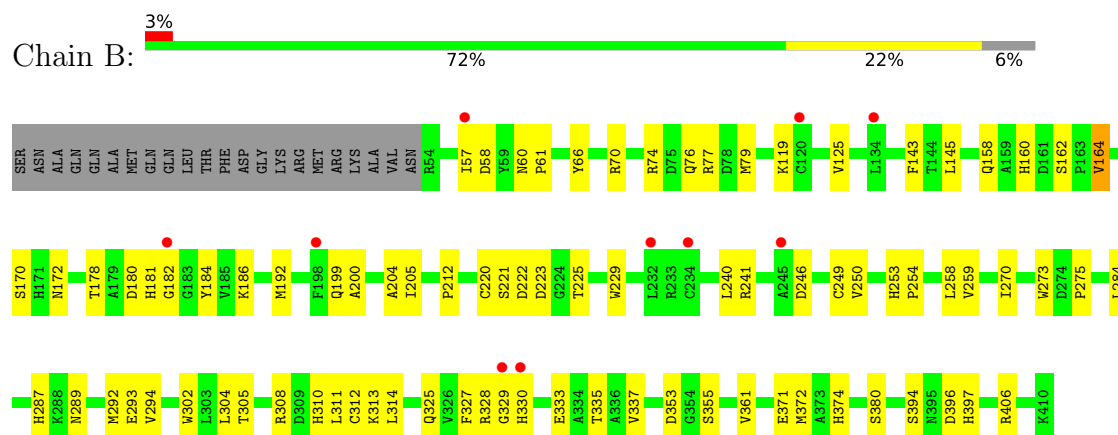
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	33	Total	O	0	0
			33	33		

These plots are drawn for all protein, RNA, 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.

- [illegible]



- 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) 100.0 (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 0.229 , 0.264	Depositor DCC
R_{free} test set	3270 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.1	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

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	0.11	0/9502	0.35	1/12903 (0.0%)
2	B	0.12	0/2955	0.35	0/4005
All	All	0.12	0/12457	0.35	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	-5.78	100.72	110.49

There are no chirality outliers.

There are no planarity outliers.

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	9290	0	9287	141	0
2	B	2872	0	2780	50	0
3	A	69	0	0	2	0
3	B	33	0	0	0	0
All	All	12264	0	12067	190	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 (190) 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
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:340:LYS:NZ	3:A:1503:HOH:O	2.33	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:374:MET:HE3	1:A:382:LEU:HD21	1.86	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: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
2:B:162:SER:OG	2:B:181:HIS:O	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:MET:HE2	1:A:586:LEU:HD21	1.89	0.55
1:A:283:VAL:HG22	1:A:323:ASP:HB3	1.90	0.54
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
2:B:76:GLN:HG3	2:B:79:MET:HE2	1.91	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:336:VAL:HG22	1:A:346:VAL:HG22	1.92	0.52
1:A:1139:ILE:HG13	1:A:1168:GLN:HG3	1.91	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:856:SER:HB3	1:A:957:GLY:HA2	1.94	0.49
1:A:1234:LEU:HD23	1:A:1245:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1282:MET:HE2	1:A:1284:LEU:HD21	1.95	0.49
1:A:521:PRO:HG3	1:A:966:MET:HE2	1.95	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:170:SER:OG	2:B:172:ASN:O	2.31	0.49
2:B:184:TYR:CE2	2:B:199:GLN:HG2	2.47	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:707:MET:HE2	1:A:707:MET:HB3	1.79	0.47
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:903:GLU:OE2	1:A:992:ARG:NH2	2.43	0.47
1:A:1183:VAL:HG11	1:A:1222:ILE:HD13	1.97	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:99:LYS:HD2	1:A:99:LYS:HA	1.66	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
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:OD1	2:B:180:ASP:N	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:991:ASN:ND2	1:A:995:GLU:HB2	2.31	0.45
1:A:1425:THR:HB	1:A:1428:ILE:HG13	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HG	1:A:1013:VAL:HG12	1.99	0.44
1:A:988:LEU:HD13	1:A:996:LEU:HD11	1.99	0.44
1:A:1311:PHE:CD1	1:A:1338:PHE:HB3	2.52	0.44
1:A:335:MET:HE2	1:A:347:LEU:HD23	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
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:894:LYS:O	1:A:1409:TYR:OH	2.33	0.44
1:A:936:ASP:OD2	1:A:985:ARG:NH1	2.51	0.44
1:A:1128:MET:HB2	2:B:61:PRO:HB3	1.99	0.44
1:A:398:GLU:H	1:A:398:GLU:HG2	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:973:ASP:OD1	1:A:973:ASP:N	2.51	0.43
1:A:1190:ILE:HG13	1:A:1208:THR:HG21	2.00	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: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:1050:MET:HB2	1:A:1054:GLU:O	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:LEU:HD11	1:A:393:LEU:HD22	2.01	0.41
1:A:354:MET:SD	1:A:354:MET:N	2.93	0.41
1:A:786:LEU:HD22	1:A:849:VAL:HG21	2.01	0.41
1:A:1287:ALA:C	1:A:1289:GLU:H	2.28	0.41
2:B:353:ASP:C	2:B:355:SER:H	2.29	0.41
1:A:670:LEU:HG	1:A:680:HIS:HB3	2.02	0.41
1:A:1379:ARG:O	1:A:1383:MET:HG2	2.20	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:600:PHE:CE1	1:A:629:LEU:HD11	2.56	0.41
1:A:1248:ARG:HG2	1:A:1294:MET:HE3	2.03	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
1:A:1407:TYR:CE2	1:A:1415:ARG:HD2	2.56	0.41
2:B:270:ILE:CD1	2:B:305:THR:HG21	2.50	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
2:B:145:LEU:HD21	2:B:192:MET:HE3	2.04	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	1009 (99%)	9 (1%)	70	87
2	B	309/327 (94%)	306 (99%)	3 (1%)	68	86
All	All	1327/1562 (85%)	1315 (99%)	12 (1%)	70	87

All (12) 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	1156	THR
1	A	1160	PHE
1	A	1299	ARG
1	A	1395	VAL
2	B	164	VAL
2	B	229	TRP
2	B	310	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN

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Mol	Chain	Res	Type
1	A	633	ASN
1	A	679	HIS
1	A	869	GLN
1	A	1334	HIS

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	1180/1443 (81%)	0.28	33 (2%) 55 50	33, 65, 108, 174	0
2	B	357/379 (94%)	0.35	10 (2%) 55 50	38, 71, 110, 139	0
All	All	1537/1822 (84%)	0.30	43 (2%) 55 50	33, 66, 108, 174	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1386	VAL	5.2
1	A	1291	PHE	4.8
2	B	330	HIS	4.2
1	A	99	LYS	3.6
2	B	198	PHE	3.6
1	A	200	LEU	3.3
1	A	535	MET	3.2
1	A	198	GLU	3.2
1	A	1051	THR	3.1
2	B	245	ALA	3.1
1	A	601	ALA	3.0
2	B	182	GLY	3.0
1	A	928	VAL	3.0
1	A	959	GLY	2.9
1	A	541	PRO	2.9
1	A	293	VAL	2.9
2	B	232	LEU	2.9
1	A	355	ARG	2.8
1	A	780	GLU	2.8
1	A	1216	ILE	2.7
1	A	89	ALA	2.6
1	A	195	ALA	2.5
1	A	247	ILE	2.5
1	A	1331	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	458	LEU	2.5
1	A	937	ILE	2.4
1	A	690	HIS	2.4
2	B	329	GLY	2.4
1	A	705	SER	2.3
1	A	1292	GLY	2.2
1	A	1290	SER	2.2
1	A	213	TYR	2.2
2	B	134	LEU	2.2
2	B	120	CYS	2.2
1	A	255	ILE	2.2
1	A	374	MET	2.1
1	A	569	GLY	2.1
1	A	710	THR	2.1
1	A	335	MET	2.1
1	A	1136	ARG	2.1
2	B	57	ILE	2.1
2	B	234	CYS	2.1
1	A	1141	ILE	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.