



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:22 PM UTC

PDB ID : 6SUP / pdb\_00006sup  
Title : Crystal Structure of TcdB2-TccC3-Cdc42  
Authors : Roderer, D.; Schubert, E.; Sitsel, O.; Raunser, S.  
Deposited on : 2019-09-16  
Resolution : 2.00 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

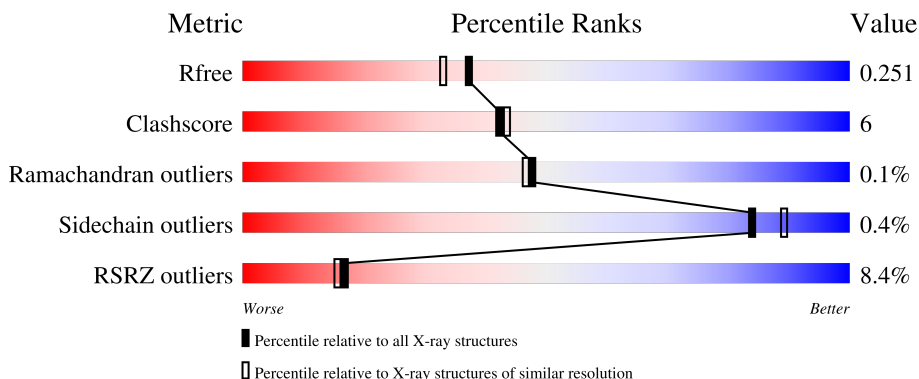
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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  $\geq 3$ , 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	2128	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18283 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 TcdB2,TccC3,Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	2128	17001	10657	3017	3294	33	1	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1017	VAL	GLY	conflict	UNP Q8GF99
A	1483	ILE	-	linker	UNP Q8GF99
A	1484	ASP	-	linker	UNP Q8GF99
A	1485	PRO	-	linker	UNP Q8GF99
A	1486	LYS	-	linker	UNP Q8GF99
A	1487	LEU	-	linker	UNP Q8GF99
A	1488	TYR	-	linker	UNP Q8GF99
A	1489	GLN	-	linker	UNP Q8GF99
A	1490	LYS	-	linker	UNP Q8GF99
A	1491	THR	-	linker	UNP Q8GF99
A	1492	PRO	-	linker	UNP Q8GF99
A	1493	THR	-	linker	UNP Q8GF99
A	1494	VAL	-	linker	UNP Q8GF99
A	1495	SER	-	linker	UNP Q8GF99
A	1496	VAL	-	linker	UNP Q8GF99
A	1497	TYR	-	linker	UNP Q8GF99
A	1498	ASP	-	linker	UNP Q8GF99
A	1499	ASN	-	linker	UNP Q8GF99
A	1500	ARG	-	linker	UNP Q8GF99
A	1501	GLY	-	linker	UNP Q8GF99
A	1502	LEU	-	linker	UNP Q8GF99
A	1503	ILE	-	linker	UNP Q8GF99
A	1504	ILE	-	linker	UNP Q8GF99
A	1505	ARG	-	linker	UNP Q8GF99
A	1506	ASN	-	linker	UNP Q8GF99
A	1507	ILE	-	linker	UNP Q8GF99
A	1508	ASP	-	linker	UNP Q8GF99

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1509	PHE	-	linker	UNP Q8GF99
A	1510	HIS	-	linker	UNP Q8GF99
A	1511	ARG	-	linker	UNP Q8GF99
A	1512	THR	-	linker	UNP Q8GF99
A	1513	THR	-	linker	UNP Q8GF99

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0

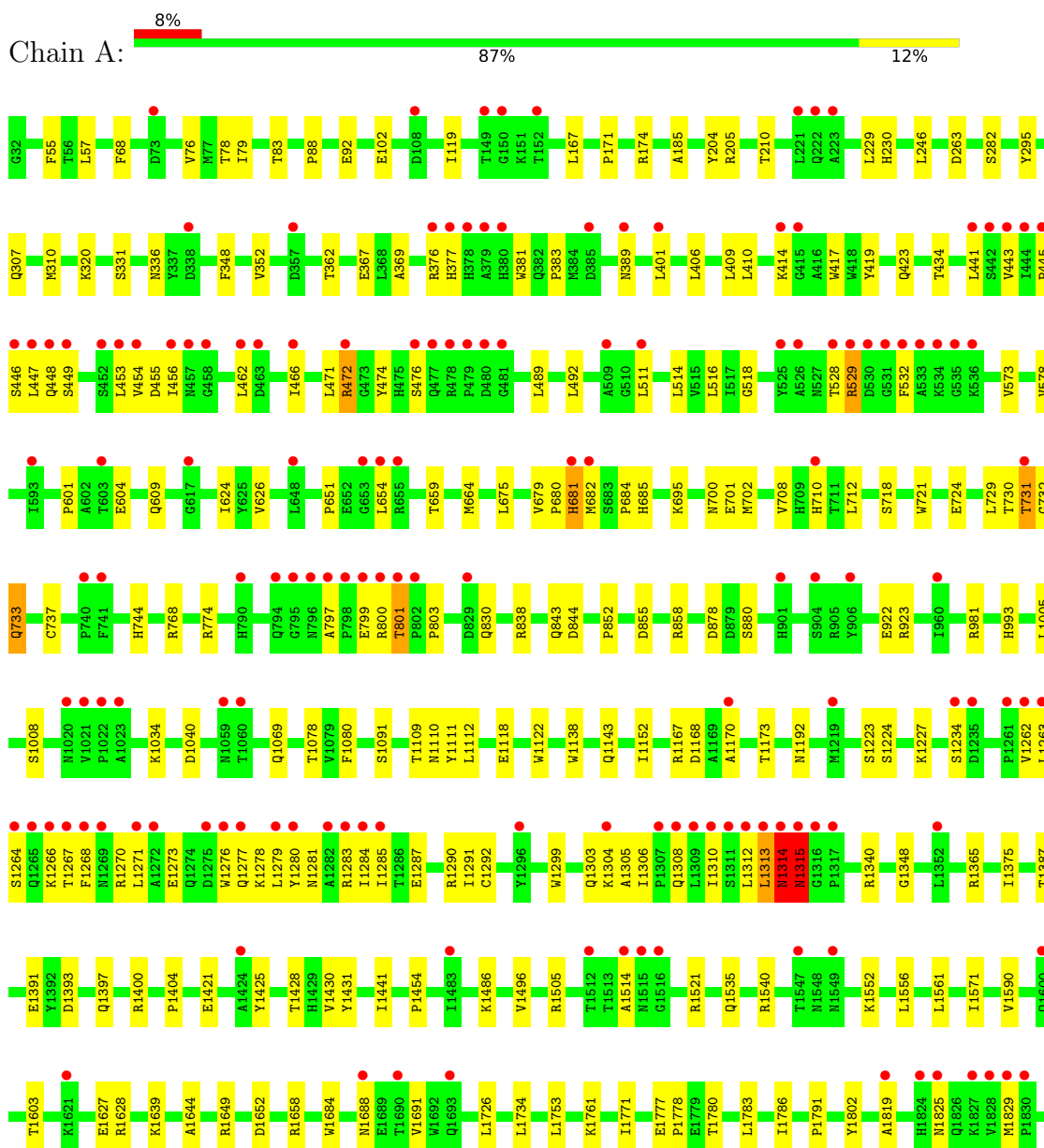
- Molecule 3 is water.

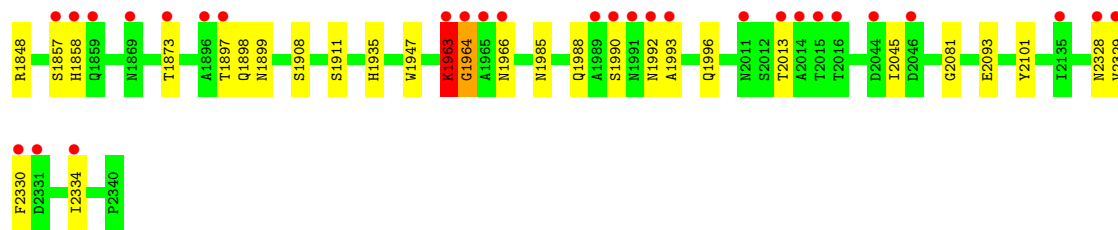
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1279	Total O 1279 1279	0	0

### 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: TcdB2,TccC3,Cell division control protein 42 homolog





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.35Å 156.55Å 179.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.00 48.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.17-2.00) 99.6 (48.17-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.287 , 0.320 0.214 , 0.251	Depositor DCC
$R_{free}$ test set	9121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtrriage
Anisotropy	0.481	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18283	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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

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	0.27	1/17420 (0.0%)	0.50	8/23750 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	803	PRO	C-O	-5.83	1.17	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	THR	CB-CA-C	-8.91	95.99	110.79
1	A	1315	ASN	N-CA-C	-7.94	103.32	113.16
1	A	681	HIS	CA-CB-CG	5.96	119.76	113.80
1	A	1964	GLY	CA-C-N	5.64	131.65	123.13
1	A	1964	GLY	C-N-CA	5.64	131.65	123.13
1	A	1963	LYS	CB-CA-C	5.55	119.46	109.64
1	A	801	THR	CB-CA-C	5.26	115.85	109.85
1	A	1314	ASN	CB-CA-C	5.12	120.61	110.42

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	17001	0	16366	210	1
2	A	3	0	0	0	0
3	A	1279	0	0	30	0
All	All	18283	0	16366	210	1

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 (210) 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:1963:LYS:HA	1:A:1963:LYS:CE	1.91	1.01
1:A:1264:SER:OG	1:A:1315:ASN:OD1	1.78	1.00
1:A:731:THR:CG2	1:A:732:GLY:N	2.31	0.94
1:A:731:THR:HG22	1:A:732:GLY:N	1.87	0.88
1:A:731:THR:CG2	1:A:732:GLY:H	1.87	0.87
1:A:731:THR:HG23	1:A:732:GLY:H	1.45	0.81
1:A:1963:LYS:HA	1:A:1963:LYS:HE2	1.65	0.78
1:A:1315:ASN:ND2	1:A:1315:ASN:H	1.82	0.77
1:A:1535:GLN:HB3	1:A:1556:LEU:HD23	1.66	0.77
1:A:1315:ASN:H	1:A:1315:ASN:HD22	1.34	0.75
1:A:401:LEU:HD22	1:A:456:ILE:HG12	1.67	0.75
1:A:695:LYS:HD2	1:A:744:HIS:CE1	2.23	0.74
1:A:1899:ASN:ND2	3:A:2509:HOH:O	2.19	0.73
1:A:453:LEU:HD23	1:A:462:LEU:HB3	1.71	0.72
1:A:1486:LYS:HD3	1:A:1514:ALA:HB1	1.71	0.72
1:A:1170:ALA:O	3:A:2502:HOH:O	2.07	0.72
1:A:880:SER:OG	3:A:2501:HOH:O	2.06	0.71
1:A:417:TRP:CD1	1:A:445:PRO:HG2	2.26	0.70
1:A:1552:LYS:NZ	3:A:2518:HOH:O	2.25	0.69
1:A:1299:TRP:HZ2	1:A:1306:ILE:HD13	1.59	0.68
1:A:1304:LYS:O	1:A:1306:ILE:HD12	1.93	0.68
1:A:1267:THR:HG21	1:A:1315:ASN:HD21	1.58	0.67
1:A:681:HIS:HB3	1:A:682:MET:HE2	1.75	0.67
1:A:852:PRO:O	3:A:2503:HOH:O	2.13	0.66
1:A:336:ASN:HB2	1:A:348:PHE:HB3	1.78	0.65
1:A:1283:ARG:NH1	3:A:2529:HOH:O	2.28	0.65
1:A:1278:LYS:HA	1:A:1281:ASN:ND2	2.11	0.65
1:A:626:VAL:N	3:A:2506:HOH:O	2.20	0.65
1:A:2045:ILE:HD11	1:A:2093:GLU:HA	1.78	0.65
1:A:352:VAL:HG22	1:A:362:THR:HG22	1.79	0.64
1:A:1278:LYS:HA	1:A:1281:ASN:HD21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:ARG:NH1	3:A:2512:HOH:O	2.21	0.64
1:A:1992:ASN:OD1	1:A:1993:ALA:N	2.30	0.63
1:A:1365:ARG:NH1	3:A:2524:HOH:O	2.27	0.63
1:A:511:LEU:HD13	1:A:514:LEU:HD21	1.80	0.63
1:A:417:TRP:HB3	1:A:441:LEU:HD13	1.80	0.62
1:A:1802:TYR:OH	3:A:2504:HOH:O	2.16	0.62
1:A:443:VAL:CG1	1:A:455:ASP:O	2.47	0.62
1:A:389:ASN:ND2	3:A:2531:HOH:O	2.31	0.61
1:A:1303:GLN:OE1	1:A:1304:LYS:HD2	2.00	0.61
1:A:858:ARG:NH1	3:A:2503:HOH:O	2.25	0.60
1:A:1306:ILE:HD12	1:A:1306:ILE:N	2.16	0.60
1:A:449:SER:HA	1:A:472:ARG:HG3	1.84	0.60
1:A:1008:SER:HB3	1:A:1112:LEU:HD13	1.82	0.60
1:A:443:VAL:HG13	1:A:455:ASP:O	2.02	0.60
1:A:843:GLN:O	3:A:2505:HOH:O	2.17	0.60
1:A:733:GLN:HA	1:A:733:GLN:OE1	2.00	0.59
1:A:1267:THR:HG21	1:A:1315:ASN:ND2	2.18	0.59
1:A:710:HIS:HB2	1:A:2330:PHE:CE1	2.37	0.59
1:A:1753:LEU:HD11	1:A:1761:LYS:HG2	1.85	0.59
1:A:1540:ARG:NH2	1:A:1908:SER:O	2.37	0.57
1:A:1963:LYS:HE2	1:A:1964:GLY:H	1.70	0.57
1:A:855:ASP:OD1	1:A:858:ARG:NH2	2.37	0.57
1:A:1304:LYS:O	1:A:1306:ILE:CD1	2.53	0.57
1:A:376:ARG:HD2	1:A:377:HIS:H	1.70	0.57
1:A:1308:GLN:CD	1:A:1308:GLN:H	2.12	0.57
1:A:609:GLN:HB3	3:A:2506:HOH:O	2.04	0.56
1:A:446:SER:O	1:A:447:LEU:HB2	2.06	0.56
1:A:476:SER:HA	1:A:528:THR:HB	1.87	0.56
1:A:609:GLN:O	3:A:2506:HOH:O	2.18	0.56
1:A:406:LEU:HG	1:A:718:SER:HB3	1.88	0.55
1:A:1305:ALA:HB1	1:A:1310:ILE:HD11	1.87	0.55
1:A:682:MET:O	1:A:685:HIS:ND1	2.39	0.55
1:A:1277:GLN:HA	1:A:1280:TYR:H	1.72	0.55
1:A:79:ILE:HD12	1:A:167:LEU:HD22	1.89	0.55
1:A:1284:ILE:HD11	1:A:1299:TRP:CG	2.43	0.54
1:A:1266:LYS:O	1:A:1270:ARG:HG3	2.07	0.53
1:A:1571:ILE:HD12	1:A:1911:SER:HA	1.90	0.53
1:A:702:MET:HE1	1:A:2334:ILE:HD11	1.89	0.53
1:A:1873:THR:HG21	1:A:1897:THR:OG1	2.08	0.53
1:A:1264:SER:CB	1:A:1315:ASN:OD1	2.55	0.53
1:A:1496:VAL:HB	1:A:1505:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:ASN:HD21	1:A:2013:THR:HG21	1.73	0.52
1:A:1167:ARG:HG2	1:A:1173:THR:HG22	1.92	0.52
1:A:922:GLU:HB2	1:A:1454:PRO:HD3	1.91	0.52
1:A:1375:ILE:HD11	1:A:1421:GLU:HG2	1.92	0.52
1:A:1935:HIS:HB3	1:A:1947:TRP:CE2	2.44	0.52
1:A:1234:SER:N	3:A:2552:HOH:O	2.40	0.52
1:A:1857:SER:OG	1:A:1858:HIS:N	2.42	0.52
1:A:1143:GLN:NE2	3:A:2543:HOH:O	2.38	0.51
1:A:1285:ILE:HD12	1:A:1291:ILE:HG12	1.92	0.51
1:A:708:VAL:HG23	1:A:1348:GLY:HA3	1.91	0.51
1:A:102:GLU:OE1	3:A:2508:HOH:O	2.19	0.51
1:A:471:LEU:HD12	1:A:471:LEU:N	2.26	0.51
1:A:981:ARG:HD3	3:A:3230:HOH:O	2.11	0.50
1:A:654:LEU:HD11	1:A:679:VAL:HG21	1.93	0.50
1:A:721:TRP:CZ2	1:A:737:CYS:HB2	2.47	0.50
1:A:1283:ARG:NH2	3:A:2573:HOH:O	2.44	0.50
1:A:1644:ALA:O	3:A:2507:HOH:O	2.18	0.50
1:A:83:THR:HG22	1:A:88:PRO:HD3	1.94	0.49
1:A:878:ASP:CG	1:A:923:ARG:HH22	2.21	0.49
1:A:401:LEU:HD11	1:A:410:LEU:HD22	1.95	0.49
1:A:1262:VAL:HG22	1:A:1290:ARG:HG2	1.93	0.49
1:A:1152:ILE:HG13	1:A:1168:ASP:HA	1.94	0.49
1:A:1271:LEU:C	1:A:1273:GLU:H	2.20	0.49
1:A:92:GLU:H	1:A:92:GLU:CD	2.19	0.49
1:A:448:GLN:HE22	1:A:454:VAL:HG23	1.77	0.49
1:A:801:THR:HG23	1:A:1431:TYR:O	2.13	0.49
1:A:1628:ARG:HG3	1:A:1684:TRP:HB2	1.95	0.49
1:A:383:PRO:HB3	1:A:684:PRO:HG2	1.95	0.49
1:A:443:VAL:HG11	1:A:455:ASP:O	2.12	0.48
1:A:1314:ASN:O	1:A:1314:ASN:ND2	2.46	0.48
1:A:376:ARG:NE	1:A:376:ARG:H	2.12	0.48
1:A:844:ASP:HB2	3:A:2505:HOH:O	2.13	0.48
1:A:417:TRP:NE1	1:A:445:PRO:HG2	2.29	0.48
1:A:369:ALA:HB3	1:A:701:GLU:HB3	1.96	0.48
1:A:1393:ASP:OD2	1:A:1397:GLN:NE2	2.35	0.48
1:A:1783:LEU:HD21	1:A:1786:ILE:HD11	1.95	0.48
1:A:1428:THR:OG1	1:A:1441:ILE:HB	2.14	0.48
1:A:185:ALA:HB1	1:A:295:TYR:CD1	2.49	0.47
1:A:993:HIS:HB2	1:A:1005:LEU:HB2	1.96	0.47
1:A:799:GLU:HB3	1:A:1430:VAL:HG21	1.96	0.47
1:A:721:TRP:CE2	1:A:737:CYS:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:GLN:HB2	1:A:1280:TYR:HB3	1.96	0.47
1:A:1091:SER:HB3	1:A:1590:VAL:HG21	1.97	0.47
1:A:1299:TRP:NE1	1:A:1304:LYS:O	2.48	0.47
1:A:774:ARG:NH1	3:A:2535:HOH:O	2.32	0.47
1:A:1540:ARG:NH1	3:A:2554:HOH:O	2.41	0.47
1:A:1306:ILE:HG23	1:A:1308:GLN:OE1	2.14	0.46
1:A:1990:SER:O	1:A:1990:SER:OG	2.16	0.46
1:A:1966:ASN:ND2	1:A:1988:GLN:NE2	2.63	0.46
1:A:528:THR:O	1:A:529:ARG:HB2	2.16	0.46
1:A:1080:PHE:HB2	1:A:1122:TRP:HB2	1.98	0.46
1:A:1848:ARG:HA	1:A:1873:THR:O	2.16	0.46
1:A:1276:TRP:CE3	1:A:1277:GLN:HB3	2.51	0.45
1:A:1726:LEU:HD22	1:A:1734:LEU:HD11	1.99	0.45
1:A:263:ASP:HB3	1:A:307:GLN:HB2	1.99	0.45
1:A:1340:ARG:NH2	3:A:2588:HOH:O	2.47	0.45
1:A:55:PHE:CZ	1:A:229:LEU:HD21	2.52	0.45
1:A:367:GLU:OE2	1:A:1292:CYS:HB3	2.16	0.45
1:A:659:THR:O	1:A:680:PRO:HG3	2.15	0.45
1:A:1223:SER:HA	1:A:1227:LYS:HZ2	1.81	0.45
1:A:1268:PHE:HA	1:A:1271:LEU:HB2	1.98	0.45
1:A:376:ARG:H	1:A:376:ARG:HE	1.63	0.45
1:A:1264:SER:OG	1:A:1267:THR:HG22	2.16	0.45
1:A:381:TRP:CD1	1:A:651:PRO:HD3	2.52	0.45
1:A:710:HIS:HB2	1:A:2330:PHE:CD1	2.52	0.45
1:A:1283:ARG:NH2	1:A:1287:GLU:H	2.15	0.45
1:A:1109:THR:HG23	1:A:1110:ASN:O	2.17	0.45
1:A:1299:TRP:CZ2	1:A:1306:ILE:HD13	2.46	0.45
1:A:1897:THR:HG22	1:A:1898:GLN:N	2.32	0.45
1:A:383:PRO:CB	1:A:684:PRO:HG2	2.47	0.45
1:A:474:TYR:CE1	1:A:476:SER:HB2	2.52	0.45
1:A:1627:GLU:HG2	1:A:1652:ASP:HA	1.99	0.45
1:A:1078:THR:HG22	1:A:1561:LEU:HD12	1.98	0.44
1:A:1111:TYR:CD1	1:A:1118:GLU:HB3	2.52	0.44
1:A:830:GLN:OE1	3:A:2511:HOH:O	2.21	0.44
1:A:1276:TRP:HE3	1:A:1277:GLN:HB3	1.82	0.44
1:A:664:MET:HE1	1:A:675:LEU:HD23	2.00	0.44
1:A:204:TYR:CE2	1:A:229:LEU:HD13	2.53	0.44
1:A:1263:LEU:HD13	1:A:1268:PHE:HD1	1.83	0.44
1:A:1649:ARG:HG2	1:A:1658:ARG:HG2	1.99	0.44
1:A:1224:SER:OG	1:A:1227:LYS:HE3	2.18	0.44
1:A:1278:LYS:HD2	1:A:1281:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1425:TYR:CE2	1:A:1778:PRO:HB2	2.53	0.43
1:A:1224:SER:H	1:A:1227:LYS:NZ	2.16	0.43
1:A:2081:GLY:HA2	1:A:2101:TYR:CD1	2.53	0.43
1:A:210:THR:CG2	1:A:282:SER:HB3	2.48	0.43
1:A:57:LEU:HD11	1:A:68:PHE:CD2	2.54	0.43
1:A:1267:THR:O	1:A:1271:LEU:HB2	2.18	0.43
1:A:2328:ASN:HB3	1:A:2329:VAL:H	1.63	0.43
1:A:1375:ILE:HG13	1:A:1421:GLU:CD	2.43	0.43
1:A:797:ALA:C	1:A:799:GLU:H	2.27	0.43
1:A:800:ARG:HD2	1:A:801:THR:H	1.84	0.43
1:A:1271:LEU:C	1:A:1273:GLU:N	2.77	0.43
1:A:1391:GLU:HB3	1:A:1400:ARG:HB2	2.00	0.43
1:A:1777:GLU:OE1	1:A:1780:THR:OG1	2.32	0.43
1:A:1780:THR:O	3:A:2510:HOH:O	2.21	0.42
1:A:320:LYS:HB2	1:A:320:LYS:HE3	1.92	0.42
1:A:624:ILE:HD13	1:A:664:MET:HE2	2.01	0.42
1:A:797:ALA:C	1:A:799:GLU:N	2.77	0.42
1:A:1312:LEU:HD22	1:A:1313:LEU:HD23	2.01	0.42
1:A:489:LEU:HD12	1:A:492:LEU:HD12	2.02	0.42
1:A:1935:HIS:HB3	1:A:1947:TRP:CD2	2.54	0.42
1:A:76:VAL:O	1:A:78:THR:HG23	2.18	0.42
1:A:573:VAL:HG13	1:A:578:VAL:HG22	2.01	0.42
1:A:729:LEU:HD23	1:A:729:LEU:O	2.20	0.42
1:A:1192:ASN:HA	1:A:1639:LYS:HG2	2.01	0.42
1:A:1771:ILE:HD12	1:A:1791:PRO:HG3	2.01	0.42
1:A:310:MET:HB3	1:A:331:SER:HB2	2.01	0.42
1:A:800:ARG:HD2	1:A:801:THR:N	2.34	0.42
1:A:1305:ALA:C	1:A:1306:ILE:HD12	2.44	0.42
1:A:1819:ALA:HB2	1:A:1829:MET:SD	2.60	0.42
1:A:409:LEU:O	1:A:419:TYR:HA	2.19	0.41
1:A:724:GLU:OE2	1:A:768:ARG:NH1	2.53	0.41
1:A:1688:ASN:O	1:A:1691:VAL:HG22	2.19	0.41
1:A:1278:LYS:CD	1:A:1281:ASN:HD21	2.33	0.41
1:A:1034:LYS:HA	1:A:1034:LYS:HD2	1.77	0.41
1:A:171:PRO:HA	1:A:174:ARG:HD3	2.03	0.41
1:A:1963:LYS:HE2	1:A:1963:LYS:CA	2.44	0.41
1:A:1985:ASN:HB3	1:A:1996:GLN:HB2	2.03	0.41
1:A:601:PRO:HB2	1:A:604:GLU:HB2	2.01	0.41
1:A:205:ARG:HG3	1:A:230:HIS:CG	2.55	0.41
1:A:1069:GLN:HG2	1:A:1138:TRP:CE2	2.55	0.41
1:A:1306:ILE:HG22	1:A:1308:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HD12	1:A:246:LEU:HD23	2.03	0.41
1:A:700:ASN:HA	1:A:712:LEU:HB2	2.02	0.41
1:A:1387:THR:HG22	1:A:1404:PRO:HB3	2.03	0.41
1:A:1963:LYS:HE2	1:A:1964:GLY:N	2.35	0.41
1:A:516:LEU:HD22	1:A:518:GLY:O	2.20	0.41
1:A:682:MET:O	1:A:685:HIS:CE1	2.74	0.41
1:A:1276:TRP:O	1:A:1279:LEU:HB2	2.21	0.41
1:A:1521:ARG:HD2	3:A:3511:HOH:O	2.21	0.41
1:A:1284:ILE:O	1:A:1292:CYS:N	2.49	0.41
1:A:529:ARG:HD2	1:A:529:ARG:HA	1.59	0.40
1:A:1552:LYS:NZ	3:A:2515:HOH:O	2.23	0.40
1:A:1963:LYS:NZ	1:A:1966:ASN:HA	2.36	0.40
1:A:1603:THR:HG23	3:A:3530:HOH:O	2.20	0.40
1:A:423:GLN:HB3	1:A:434:THR:HG23	2.03	0.40
1:A:466:ILE:HG12	1:A:471:LEU:HD21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:ASP:OD1	1:A:1825:ASN:ND2[1_655]	2.08	0.12

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	2122/2128 (100%)	2060 (97%)	59 (3%)	3 (0%)	48 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	532	PHE

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Mol	Chain	Res	Type
1	A	529	ARG
1	A	414	LYS

### 5.3.2 Protein sidechains [i](#)

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	1840/1840 (100%)	1833 (100%)	7 (0%)	<a href="#">84</a> <a href="#">89</a>

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	ARG
1	A	731	THR
1	A	733	GLN
1	A	1313	LEU
1	A	1314	ASN
1	A	1315	ASN
1	A	1963	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	75	ASN
1	A	371	GLN
1	A	498	HIS
1	A	845	ASN
1	A	1050	GLN
1	A	1082	GLN
1	A	1165	GLN
1	A	1314	ASN
1	A	1394	ASN
1	A	1534	ASN
1	A	1546	GLN

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Mol	Chain	Res	Type
1	A	1564	ASN
1	A	1747	GLN
1	A	1781	GLN
1	A	1869	ASN
1	A	1987	GLN
1	A	1988	GLN
1	A	1996	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2157:LEU	C	2328:ASN	N	47.21
1	A	1471:LYS	C	1483:ILE	N	13.98

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	2128/2128 (100%)	0.43	179 (8%) <b>17</b> <b>15</b>	22, 36, 81, 145	1 (0%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	PRO	8.0
1	A	1263	LEU	7.4
1	A	1276	TRP	5.9
1	A	1829	MET	5.8
1	A	1023	ALA	5.5
1	A	1989	ALA	5.5
1	A	532	PHE	5.3
1	A	444	ILE	5.2
1	A	2014	ALA	5.1
1	A	456	ILE	5.0
1	A	1280	TYR	5.0
1	A	2330	PHE	4.8
1	A	797	ALA	4.8
1	A	1483	ILE	4.8
1	A	533	ALA	4.7
1	A	2015	THR	4.6
1	A	1262	VAL	4.6
1	A	462	LEU	4.5
1	A	1310	ILE	4.3
1	A	1272	ALA	4.2
1	A	529	ARG	4.1
1	A	1271	LEU	4.1
1	A	442	SER	4.0
1	A	108	ASP	4.0
1	A	443	VAL	3.9
1	A	2329	VAL	3.9
1	A	654	LEU	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	535	GLY	3.8
1	A	1282	ALA	3.8
1	A	453	LEU	3.8
1	A	1269	ASN	3.8
1	A	802	PRO	3.7
1	A	1021	VAL	3.7
1	A	457	ASN	3.7
1	A	1268	PHE	3.7
1	A	1965	ALA	3.7
1	A	801	THR	3.7
1	A	1283	ARG	3.7
1	A	1312	LEU	3.7
1	A	682	MET	3.7
1	A	472	ARG	3.7
1	A	454	VAL	3.6
1	A	681	HIS	3.6
1	A	1858	HIS	3.4
1	A	528	THR	3.4
1	A	1275	ASP	3.4
1	A	795	GLY	3.4
1	A	534	LYS	3.4
1	A	477	GLN	3.3
1	A	531	GLY	3.3
1	A	653	GLY	3.3
1	A	377	HIS	3.3
1	A	447	LEU	3.3
1	A	509	ALA	3.2
1	A	1992	ASN	3.2
1	A	446	SER	3.2
1	A	1515	ASN	3.2
1	A	530	ASP	3.2
1	A	731	THR	3.2
1	A	794	GLN	3.1
1	A	1964	GLY	3.1
1	A	2016	THR	3.1
1	A	479	PRO	3.1
1	A	2013	THR	3.0
1	A	1830	PRO	3.0
1	A	379	ALA	3.0
1	A	1313	LEU	3.0
1	A	1690	THR	3.0
1	A	798	PRO	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1317	PRO	3.0
1	A	2331	ASP	3.0
1	A	481	GLY	3.0
1	A	1267	THR	3.0
1	A	796	ASN	3.0
1	A	960	ILE	3.0
1	A	1279	LEU	2.9
1	A	338	ASP	2.9
1	A	1059	ASN	2.9
1	A	1296	TYR	2.9
1	A	449	SER	2.9
1	A	1990	SER	2.9
1	A	152	THR	2.9
1	A	466	ILE	2.9
1	A	414	LYS	2.9
1	A	376	ARG	2.8
1	A	800	ARG	2.8
1	A	1308	GLN	2.8
1	A	1828	VAL	2.8
1	A	441	LEU	2.8
1	A	1022	PRO	2.8
1	A	480	ASP	2.8
1	A	1170	ALA	2.8
1	A	1869	ASN	2.7
1	A	1316	GLY	2.7
1	A	1896	ALA	2.7
1	A	1020	ASN	2.7
1	A	476	SER	2.7
1	A	458	GLY	2.7
1	A	448	GLN	2.6
1	A	1827	LYS	2.6
1	A	150	GLY	2.6
1	A	222	GLN	2.6
1	A	710	HIS	2.6
1	A	1963	LYS	2.6
1	A	1264	SER	2.6
1	A	1693	GLN	2.5
1	A	525	TYR	2.5
1	A	1825	ASN	2.5
1	A	1966	ASN	2.5
1	A	1991	ASN	2.5
1	A	1235	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1859	GLN	2.5
1	A	2044	ASP	2.5
1	A	741	PHE	2.5
1	A	415	GLY	2.5
1	A	149	THR	2.4
1	A	1261	PRO	2.4
1	A	1352	LEU	2.4
1	A	1284	ILE	2.4
1	A	603	THR	2.4
1	A	536	LYS	2.4
1	A	478	ARG	2.4
1	A	1266	LYS	2.4
1	A	221	LEU	2.3
1	A	1549	ASN	2.3
1	A	452	SER	2.3
1	A	1311	SER	2.3
1	A	1824	HIS	2.3
1	A	1688	ASN	2.3
1	A	648	LEU	2.3
1	A	380	HIS	2.2
1	A	1873	THR	2.2
1	A	1897	THR	2.2
1	A	357	ASP	2.2
1	A	829	ASP	2.2
1	A	1219	MET	2.2
1	A	799	GLU	2.2
1	A	901	HIS	2.2
1	A	2046	ASP	2.2
1	A	1516	GLY	2.2
1	A	906	TYR	2.2
1	A	1304	LYS	2.2
1	A	2011	ASN	2.2
1	A	1060	THR	2.2
1	A	1307	PRO	2.2
1	A	1277	GLN	2.2
1	A	1857	SER	2.2
1	A	1315	ASN	2.2
1	A	463	ASP	2.2
1	A	1547	THR	2.2
1	A	617	GLY	2.1
1	A	1819	ALA	2.1
1	A	1993	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	593	ILE	2.1
1	A	1600	GLN	2.1
1	A	2334	ILE	2.1
1	A	655	ARG	2.1
1	A	1514	ALA	2.1
1	A	1314	ASN	2.1
1	A	2328	ASN	2.1
1	A	73	ASP	2.1
1	A	740	PRO	2.1
1	A	1265	GLN	2.1
1	A	2135	ILE	2.1
1	A	401	LEU	2.1
1	A	389	ASN	2.1
1	A	378	HIS	2.1
1	A	1512	THR	2.1
1	A	1285	ILE	2.1
1	A	223	ALA	2.1
1	A	1234	SER	2.1
1	A	1424	ALA	2.1
1	A	511	LEU	2.0
1	A	1621	LYS	2.0
1	A	904	SER	2.0
1	A	526	ALA	2.0
1	A	1309	LEU	2.0
1	A	385	ASP	2.0
1	A	790	HIS	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, 95<sup>th</sup> 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
2	MG	A	2401	1/1	0.95	0.09	41,41,41,41	0
2	MG	A	2403	1/1	0.95	0.06	32,32,32,32	0
2	MG	A	2402	1/1	0.98	0.06	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.