



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:07 am BST

PDB ID : 5W94  
Title : Crystal structure of Scc4 in complex with Scc2n and Ctf19n  
Authors : Hinshaw, S.M.; Harrison, S.C.  
Deposited on : 2017-06-22  
Resolution : 3.19 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

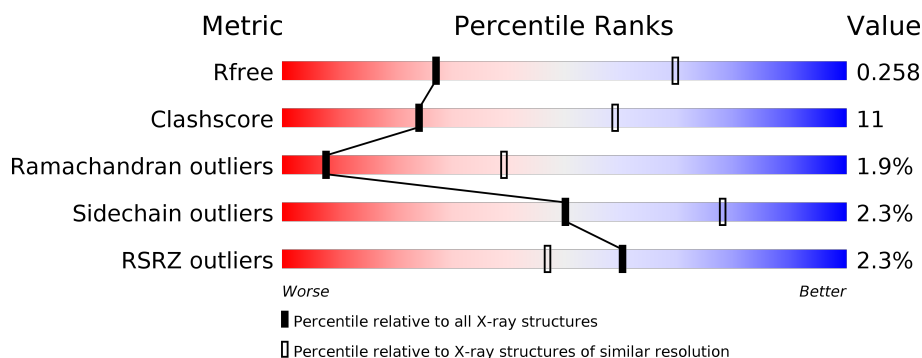
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	624	<div> <div>8%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	C	624	<div> <div>76%</div> <div>19%</div> <div>..</div> </div>
2	B	184	<div> <div>3%</div> <div>36%</div> <div>23%</div> <div>..</div> <div>38%</div> </div>
2	D	184	<div> <div>8%</div> <div>44%</div> <div>15%</div> <div>.</div> <div>40%</div> </div>
3	E	6	<div> <div>33%</div> <div>50%</div> <div>17%</div> <div>33%</div> </div>
3	H	6	<div> <div>50%</div> <div>17%</div> <div>33%</div> </div>

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	TPO	E	4	-	-	-	X
3	SEP	E	5	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11738 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 MAU2 chromatid cohesion factor homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	617	Total	C	N	O	S	0	0	0
			5008	3216	840	915	37			
1	C	605	Total	C	N	O	S	0	0	0
			4928	3168	826	897	37			

- Molecule 2 is a protein called Sister chromatid cohesion protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	114	Total	C	N	O	S	0	0	0
			874	553	150	170	1			
2	D	110	Total	C	N	O	S	0	0	0
			848	541	144	162	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP Q04002
B	-1	ASN	-	expression tag	UNP Q04002
B	0	ALA	-	expression tag	UNP Q04002
D	-2	SER	-	expression tag	UNP Q04002
D	-1	ASN	-	expression tag	UNP Q04002
D	0	ALA	-	expression tag	UNP Q04002

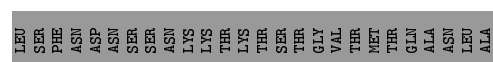
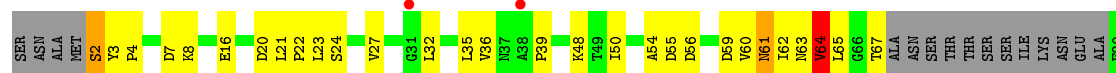
- Molecule 3 is a protein called Ctf19n.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	P	0	0	0
			40	20	4	14	2			
3	H	4	Total	C	N	O	P	0	0	0
			40	20	4	14	2			

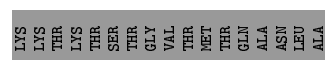
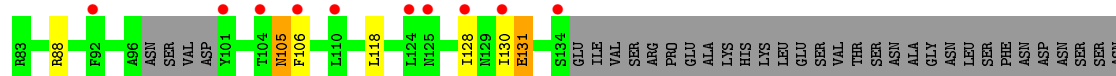
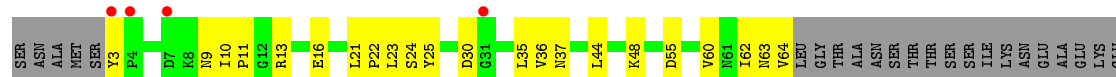
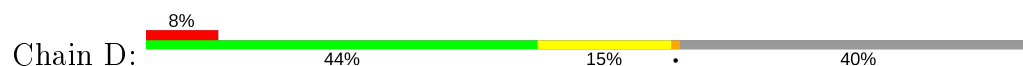




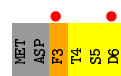
• Molecule 2: Sister chromatid cohesion protein 2



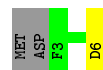
• Molecule 2: Sister chromatid cohesion protein 2



• Molecule 3: Ctf19n



• Molecule 3: Ctf19n



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.97Å 172.97Å 145.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.94 – 3.19 39.94 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.94-3.19) 99.1 (39.94-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.209 , 0.258 0.209 , 0.258	Depositor DCC
$R_{free}$ test set	1996 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.6	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.60	0/5107	0.79	4/6888 (0.1%)
1	C	0.47	0/5025	0.70	2/6775 (0.0%)
2	B	0.61	0/887	0.92	0/1198
2	D	0.46	0/863	0.71	0/1169
3	E	0.49	0/18	0.33	0/21
3	H	0.48	0/18	0.65	0/21
All	All	0.54	0/11918	0.76	6/16072 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LEU	CA-CB-CG	5.54	128.05	115.30
1	C	390	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	305	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	A	123	LEU	CA-CB-CG	5.29	127.47	115.30
1	C	305	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	A	500	TRP	CA-CB-CG	5.02	123.24	113.70

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	5008	0	5059	138	1
1	C	4928	0	4986	89	0
2	B	874	0	885	52	1
2	D	848	0	864	22	1
3	E	40	0	21	2	0
3	H	40	0	22	0	0
All	All	11738	0	11837	259	2

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 11.

All (259) 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:65:LEU:HD11	2:B:121:HIS:CD2	1.49	1.45
2:B:65:LEU:CD1	2:B:121:HIS:HD2	1.42	1.30
2:B:65:LEU:CD1	2:B:121:HIS:CD2	2.22	1.18
1:A:6:ASP:O	1:A:7:LYS:HG3	1.53	1.08
2:B:61:ASN:ND2	2:B:63:ASN:OD1	1.99	0.93
1:A:6:ASP:OD1	2:B:63:ASN:OD1	1.87	0.92
1:A:318:TYR:OH	1:A:541:LYS:O	1.93	0.85
2:B:65:LEU:HD12	2:B:121:HIS:HD2	1.42	0.84
1:A:616:VAL:HG12	2:B:8:LYS:NZ	1.96	0.79
1:A:6:ASP:OD1	2:B:61:ASN:ND2	2.16	0.79
1:A:616:VAL:HG12	2:B:8:LYS:HZ3	1.47	0.79
1:A:320:GLU:HG2	1:A:321:LYS:H	1.49	0.77
1:A:525:LYS:O	1:A:527:VAL:N	2.15	0.76
1:A:491:LEU:HD12	1:A:552:LEU:HD21	1.67	0.75
1:C:483:GLU:OE2	1:C:536:ARG:NH1	2.21	0.74
1:C:8:LEU:HD12	2:D:62:ILE:HG21	1.67	0.74
1:C:555:ARG:HD3	1:C:591:TRP:NE1	2.02	0.73
1:A:465:LEU:HD23	1:A:468:GLU:HG3	1.72	0.72
1:A:616:VAL:CG1	2:B:8:LYS:HD2	2.20	0.71
1:C:53:LEU:HD11	2:D:64:VAL:HG13	1.71	0.70
1:A:73:VAL:HG11	1:A:90:ILE:HD11	1.74	0.69
2:B:88:ARG:HB3	2:B:131:GLU:HB2	1.73	0.69
1:A:84:ASP:OD1	1:A:125:ARG:NH2	2.26	0.69
1:C:616:VAL:O	1:C:620:THR:OG1	2.12	0.67
2:B:128:ILE:HD11	2:B:130:ILE:HD11	1.76	0.67
1:C:560:ASP:HB3	1:C:563:GLU:HG3	1.77	0.67
1:C:173:GLN:OE1	1:C:176:ARG:NH1	2.26	0.67
1:C:27:ILE:HD13	2:D:106:PHE:HD2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:MET:HG2	1:C:284:PRO:HD2	1.77	0.66
1:C:84:ASP:OD1	1:C:125:ARG:NH2	2.29	0.65
1:A:6:ASP:CG	2:B:63:ASN:OD1	2.35	0.64
1:A:27:ILE:HG21	2:B:106:PHE:HB3	1.80	0.64
1:C:112:ARG:NE	2:D:44:LEU:O	2.30	0.63
1:A:283:MET:HE3	1:A:284:PRO:HD2	1.81	0.62
1:C:27:ILE:HD13	2:D:106:PHE:CD2	2.34	0.62
1:A:269:SER:O	1:A:273:ASN:HB3	1.99	0.62
1:A:21:ARG:HG3	1:A:75:LEU:HD21	1.81	0.62
3:E:5:SEP:OG	3:E:6:ASP:N	2.33	0.61
1:A:6:ASP:O	1:A:7:LYS:CG	2.39	0.61
1:A:387:SER:O	1:A:389:LYS:N	2.34	0.61
1:A:398:ARG:HG3	1:A:419:LEU:HD13	1.83	0.61
2:B:130:ILE:HG22	2:B:131:GLU:H	1.65	0.61
1:A:373:TRP:CD1	2:B:27:VAL:HG22	2.36	0.60
1:C:67:LYS:HE3	2:D:48:LYS:O	2.01	0.60
1:A:203:VAL:HG11	1:A:221:LEU:HD22	1.83	0.60
1:A:464:TRP:NE1	1:A:468:GLU:OE2	2.33	0.60
2:B:65:LEU:HA	2:B:124:LEU:HD11	1.85	0.59
1:C:492:PHE:HE1	1:C:552:LEU:HD13	1.68	0.58
2:B:65:LEU:HD12	2:B:121:HIS:CD2	2.22	0.58
1:C:491:LEU:HD12	1:C:552:LEU:HD21	1.86	0.58
1:A:20:TYR:OH	2:B:114:ALA:O	2.21	0.58
1:A:385:THR:HG22	1:A:386:GLU:H	1.69	0.58
1:A:363:ILE:HG12	2:B:35:LEU:HD21	1.86	0.58
1:C:419:LEU:HD12	1:C:425:THR:HG21	1.84	0.58
1:A:373:TRP:NE1	2:B:27:VAL:HG22	2.19	0.57
1:C:73:VAL:HG21	1:C:90:ILE:HD11	1.86	0.57
1:A:4:LEU:HD11	1:A:7:LYS:N	2.20	0.57
1:C:20:TYR:HB2	1:C:47:SER:HB2	1.87	0.56
1:A:399:LEU:HD22	1:A:429:VAL:HG13	1.86	0.56
2:B:22:PRO:O	2:B:24:SER:N	2.38	0.56
2:B:62:ILE:O	2:B:62:ILE:HG13	2.02	0.56
1:A:67:LYS:HE3	2:B:48:LYS:O	2.05	0.56
1:A:484:CYS:HB2	1:A:520:PHE:CE1	2.40	0.55
1:A:384:THR:HG23	1:A:385:THR:H	1.72	0.55
1:A:321:LYS:O	1:A:324:PHE:HB3	2.06	0.55
1:C:412:ALA:HA	1:C:415:GLU:HG2	1.88	0.55
1:A:616:VAL:HG11	2:B:8:LYS:HD2	1.89	0.55
1:C:210:ARG:HD2	1:C:475:ASP:OD2	2.07	0.54
2:D:22:PRO:O	2:D:24:SER:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:HG3	1:A:156:TRP:CD2	2.41	0.54
1:A:455:GLU:O	1:A:458:GLU:HB3	2.07	0.54
1:A:77:ILE:HG23	1:A:124:MET:HG3	1.89	0.54
1:A:372:VAL:HG13	1:A:383:VAL:HG22	1.89	0.54
1:C:177:VAL:O	1:C:181:PHE:HB2	2.08	0.54
1:C:363:ILE:HG12	2:D:35:LEU:HD21	1.89	0.54
1:C:447:ARG:HB3	2:D:16:GLU:OE2	2.08	0.54
1:C:55:LYS:NZ	1:C:65:ASP:OD1	2.41	0.53
1:A:77:ILE:HD11	1:A:121:LEU:HG	1.89	0.53
2:D:128:ILE:HD11	2:D:130:ILE:HD11	1.91	0.53
1:C:210:ARG:NH1	1:C:475:ASP:OD2	2.36	0.53
1:A:518:ARG:NH1	1:A:557:LEU:HD22	2.24	0.53
1:A:573:ASP:O	1:A:576:ARG:HG2	2.08	0.53
1:A:81:TYR:CZ	2:B:87:LYS:HG2	2.43	0.53
1:A:111:MET:HG3	1:A:156:TRP:CE2	2.44	0.53
1:A:4:LEU:HD13	1:A:5:GLY:N	2.24	0.53
1:C:333:TYR:CE2	1:C:368:GLU:HG2	2.44	0.53
1:C:188:CYS:HB3	1:C:195:LYS:HB2	1.90	0.52
1:A:73:VAL:HG21	1:A:90:ILE:HD11	1.91	0.52
1:A:53:LEU:HD23	2:B:62:ILE:HG22	1.90	0.52
1:C:497:PRO:HA	2:D:13:ARG:NH1	2.25	0.52
1:C:573:ASP:O	1:C:576:ARG:HG2	2.10	0.52
1:C:398:ARG:HG3	1:C:419:LEU:HD13	1.92	0.52
1:C:488:ILE:HD11	1:C:549:VAL:HG22	1.92	0.52
1:A:382:VAL:HG12	1:A:384:THR:H	1.75	0.51
1:A:542:ALA:HB3	1:A:545:LEU:HB3	1.92	0.51
1:A:616:VAL:CG1	2:B:8:LYS:NZ	2.72	0.51
1:A:472:GLN:O	1:A:477:GLN:NE2	2.44	0.51
1:C:492:PHE:CE1	1:C:552:LEU:HD13	2.45	0.51
1:A:388:PRO:O	1:A:389:LYS:HD3	2.10	0.51
1:C:465:LEU:HD23	1:C:468:GLU:HG3	1.91	0.51
1:A:219:GLN:HG2	1:A:222:ARG:HH21	1.76	0.51
1:C:263:PHE:CE2	1:C:302:LYS:HD3	2.46	0.51
1:A:317:CYS:SG	1:A:378:LEU:HB2	2.51	0.51
1:A:481:ILE:HG23	1:A:545:LEU:HD22	1.93	0.51
1:A:69:THR:HB	1:A:93:LEU:HD22	1.92	0.51
2:B:65:LEU:HG	2:B:124:LEU:HG	1.93	0.50
1:C:565:TYR:CZ	1:C:601:ARG:HD3	2.47	0.50
1:A:359:THR:OG1	2:B:39:PRO:HD3	2.11	0.50
1:A:366:PHE:CE1	1:A:392:PRO:HB2	2.47	0.50
1:A:540:LYS:O	1:A:542:ALA:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ILE:HD11	1:C:288:LEU:HD12	1.92	0.50
1:A:111:MET:HE2	1:A:156:TRP:HB3	1.93	0.49
1:A:518:ARG:HG3	1:A:557:LEU:HD13	1.93	0.49
1:C:191:LYS:HG2	1:C:196:TRP:CZ2	2.47	0.49
1:A:14:TYR:CE1	2:B:50:ILE:HD11	2.47	0.49
1:A:525:LYS:C	1:A:527:VAL:H	2.11	0.49
1:A:555:ARG:HD3	1:A:591:TRP:NE1	2.28	0.49
1:A:551:TYR:CD1	1:A:588:ILE:HD13	2.47	0.49
1:C:77:ILE:HG23	1:C:124:MET:HG3	1.94	0.49
1:C:321:LYS:O	1:C:324:PHE:HB3	2.13	0.49
1:A:447:ARG:HB3	2:B:16:GLU:OE2	2.12	0.49
1:A:391:GLY:O	1:A:393:SER:N	2.46	0.48
1:A:4:LEU:HD22	1:A:5:GLY:H	1.77	0.48
1:C:543:LEU:HD22	1:C:577:GLN:HB2	1.94	0.48
1:A:119:HIS:HD2	1:A:163:VAL:HG22	1.78	0.48
1:A:73:VAL:HG21	1:A:90:ILE:CD1	2.43	0.48
1:C:86:ALA:O	1:C:90:ILE:HG12	2.12	0.48
1:C:614:ALA:HA	1:C:617:LYS:HE3	1.94	0.48
1:A:4:LEU:HD21	1:A:7:LYS:HB2	1.96	0.48
2:B:111:SER:O	2:B:115:GLN:HG3	2.13	0.48
1:C:165:VAL:HG11	1:C:181:PHE:CE2	2.48	0.48
1:A:391:GLY:C	1:A:393:SER:H	2.16	0.48
1:A:593:LEU:HD11	1:A:605:VAL:HG13	1.95	0.48
1:A:5:GLY:O	1:A:6:ASP:HB2	2.14	0.48
1:A:119:HIS:CD2	1:A:163:VAL:HG22	2.49	0.48
1:A:111:MET:CE	1:A:156:TRP:HB3	2.44	0.47
1:A:295:ILE:HD11	2:B:36:VAL:HA	1.96	0.47
1:C:73:VAL:HG21	1:C:90:ILE:CD1	2.44	0.47
1:A:303:ASN:OD1	1:A:336:THR:OG1	2.32	0.47
1:A:495:PHE:CE1	1:A:510:ARG:HG2	2.50	0.47
1:A:384:THR:CG2	1:A:404:LYS:HE3	2.45	0.47
1:C:173:GLN:OE1	1:C:176:ARG:HD3	2.15	0.47
1:C:428:GLU:O	1:C:431:MET:N	2.47	0.47
1:C:283:MET:HE2	1:C:284:PRO:O	2.15	0.47
1:C:316:ASN:HB3	1:C:319:ASP:OD1	2.15	0.47
2:D:88:ARG:HG2	2:D:131:GLU:HG2	1.96	0.47
1:A:488:ILE:HD11	1:A:549:VAL:HG22	1.96	0.46
1:C:391:GLY:CA	1:C:397:VAL:HG23	2.44	0.46
1:C:589:GLY:O	1:C:593:LEU:N	2.45	0.46
1:A:477:GLN:HG3	1:A:478:PHE:CE1	2.50	0.46
1:A:320:GLU:O	1:A:323:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLY:HA3	1:A:347:GLY:HA2	1.77	0.46
1:A:318:TYR:CE2	1:A:543:LEU:HB2	2.50	0.46
1:C:25:TYR:O	1:C:345:ALA:HB1	2.16	0.46
1:C:572:PHE:CE1	1:C:585:GLN:HG2	2.51	0.46
1:A:270:LEU:O	1:A:274:GLU:HB2	2.16	0.46
3:E:3:PHE:HD1	3:E:4:TPO:N	2.14	0.46
1:C:9:SER:N	1:C:12:GLN:OE1	2.46	0.45
1:A:500:TRP:CD1	2:B:16:GLU:OE2	2.69	0.45
1:C:601:ARG:O	1:C:605:VAL:HG23	2.15	0.45
1:A:616:VAL:CG1	2:B:8:LYS:CD	2.93	0.45
1:C:377:LEU:HD23	1:C:377:LEU:HA	1.79	0.45
1:A:27:ILE:O	1:A:31:ILE:HD12	2.17	0.45
1:C:444:ARG:O	1:C:448:CYS:HB2	2.16	0.45
1:A:316:ASN:O	1:A:318:TYR:N	2.50	0.45
1:A:560:ASP:HB3	1:A:563:GLU:HG3	1.99	0.45
1:A:616:VAL:HG13	2:B:8:LYS:HD2	1.95	0.45
1:A:300:GLU:HG3	1:A:339:LEU:HD13	1.99	0.45
1:A:29:ASN:HA	2:B:93:THR:HB	1.99	0.45
1:C:555:ARG:HG2	1:C:591:TRP:CZ2	2.52	0.45
1:A:216:ASP:OD1	1:A:216:ASP:N	2.50	0.44
1:A:4:LEU:CD1	1:A:6:ASP:H	2.31	0.44
1:C:472:GLN:O	1:C:477:GLN:NE2	2.50	0.44
1:C:464:TRP:CH2	1:C:486:VAL:HG13	2.53	0.44
1:A:282:ILE:HD11	1:A:288:LEU:HD12	2.00	0.44
1:A:607:LEU:O	1:A:610:ALA:N	2.50	0.44
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.78	0.44
1:C:596:CYS:HB3	1:C:605:VAL:HG22	2.00	0.44
2:B:32:LEU:HA	2:B:32:LEU:HD23	1.78	0.44
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.77	0.44
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.83	0.44
2:D:88:ARG:HB3	2:D:131:GLU:HA	2.00	0.44
1:C:101:GLN:O	1:C:103:ASP:N	2.51	0.44
1:A:419:LEU:HD12	1:A:425:THR:HG21	1.98	0.44
1:A:4:LEU:HD13	1:A:6:ASP:H	1.83	0.44
1:A:53:LEU:HA	1:A:53:LEU:HD12	1.66	0.44
1:C:390:LEU:HB3	1:C:391:GLY:H	1.65	0.44
1:A:124:MET:HB3	1:A:124:MET:HE3	1.77	0.43
1:A:373:TRP:HE1	2:B:27:VAL:HG22	1.82	0.43
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.78	0.43
2:B:64:VAL:HB	2:B:65:LEU:H	1.39	0.43
1:A:81:TYR:CE1	2:B:87:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:HG2	1:A:342:ASN:OD1	2.18	0.43
1:A:90:ILE:HG23	1:A:90:ILE:HD12	1.74	0.43
2:B:21:LEU:HA	2:B:21:LEU:HD12	1.63	0.43
1:C:477:GLN:HG3	1:C:478:PHE:CE1	2.54	0.43
2:B:132:LYS:HE2	2:B:132:LYS:HB3	1.65	0.43
2:D:10:ILE:HG23	2:D:11:PRO:HD2	2.00	0.43
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.76	0.43
1:A:318:TYR:CD1	1:A:318:TYR:O	2.72	0.43
1:A:477:GLN:HG3	1:A:478:PHE:CD1	2.53	0.43
2:B:20:ASP:OD1	2:B:20:ASP:N	2.48	0.43
1:C:391:GLY:HA2	1:C:397:VAL:HG23	2.01	0.43
1:C:295:ILE:HD11	2:D:36:VAL:HG13	2.01	0.42
1:C:395:GLY:HA2	1:C:398:ARG:HE	1.84	0.42
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.75	0.42
2:B:59:ASP:N	2:B:59:ASP:OD1	2.52	0.42
1:C:123:LEU:HA	1:C:123:LEU:HD23	1.85	0.42
1:A:145:MET:HE2	1:A:145:MET:HB3	1.72	0.42
1:A:4:LEU:HD11	1:A:7:LYS:C	2.39	0.42
1:C:463:VAL:O	1:C:467:VAL:HG23	2.19	0.42
1:C:491:LEU:CD1	1:C:517:LEU:HD22	2.49	0.42
1:A:445:VAL:HG13	1:A:453:GLN:HE21	1.84	0.42
1:A:574:MET:O	1:A:576:ARG:N	2.52	0.42
1:A:447:ARG:HB3	2:B:16:GLU:CD	2.40	0.42
1:C:481:ILE:HD11	1:C:540:LYS:HB2	2.01	0.42
1:A:23:HIS:HD2	1:A:43:LEU:HD11	1.85	0.42
1:C:484:CYS:HA	1:C:520:PHE:CE2	2.55	0.42
1:A:544:LEU:HD12	1:A:544:LEU:HA	1.80	0.42
1:C:317:CYS:SG	1:C:378:LEU:HB2	2.60	0.42
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.93	0.42
1:A:614:ALA:O	1:A:618:GLN:HG3	2.20	0.42
1:A:547:ILE:HD11	1:A:574:MET:HB2	2.00	0.42
2:B:3:TYR:HB2	2:B:4:PRO:HD2	2.01	0.42
1:C:346:GLY:HA3	1:C:347:GLY:HA2	1.67	0.42
1:A:13:VAL:HG21	2:B:60:VAL:HB	2.02	0.41
1:C:580:GLY:O	2:D:21:LEU:HD13	2.20	0.41
1:A:183:GLY:O	1:A:187:GLN:NE2	2.28	0.41
1:A:369:PHE:CZ	1:A:396:TYR:CD2	3.08	0.41
1:A:609:ASN:O	1:A:613:GLU:HG3	2.20	0.41
2:B:54:ALA:C	2:B:56:ASP:H	2.23	0.41
1:C:8:LEU:O	2:D:60:VAL:N	2.47	0.41
1:A:496:GLU:HG3	1:A:502:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD22	1:A:64:GLU:HB3	2.01	0.41
1:A:449:SER:O	1:A:453:GLN:HB2	2.19	0.41
2:B:113:LEU:O	2:B:117:VAL:HG23	2.20	0.41
1:C:398:ARG:HG2	1:C:398:ARG:H	1.73	0.41
1:C:545:LEU:HB2	2:D:25:TYR:CE2	2.55	0.41
2:B:110:LEU:HD23	2:B:110:LEU:HA	1.84	0.41
1:C:101:GLN:HG3	1:C:102:SER:N	2.35	0.41
1:C:395:GLY:HA2	1:C:398:ARG:HG2	2.03	0.41
1:C:545:LEU:HB2	2:D:25:TYR:CD2	2.56	0.41
1:A:420:ALA:HA	1:A:430:LYS:HG2	2.03	0.41
1:C:72:MET:HE1	1:C:89:TYR:CZ	2.56	0.41
1:C:318:TYR:CE2	1:C:543:LEU:HB2	2.56	0.41
2:D:44:LEU:HD12	2:D:44:LEU:HA	1.60	0.41
1:A:411:GLY:HA3	1:A:444:ARG:NH2	2.36	0.40
1:C:73:VAL:HG13	1:C:86:ALA:HB1	2.04	0.40
1:C:46:MET:HG3	2:D:118:LEU:HD13	2.03	0.40
1:A:118:LEU:HD13	1:A:138:CYS:HA	2.03	0.40
1:A:35:GLU:O	1:A:38:LYS:N	2.54	0.40
1:A:383:VAL:O	1:A:385:THR:N	2.54	0.40
1:A:471:LEU:O	1:A:477:GLN:HB3	2.21	0.40
1:C:480:PRO:HB2	1:C:539:LEU:HD23	2.03	0.40
1:C:542:ALA:HB3	1:C:545:LEU:HB3	2.03	0.40
1:C:426:SER:HB3	2:D:30:ASP:CG	2.42	0.40
1:A:386:GLU:HB2	1:A:387:SER:H	1.48	0.40
1:A:603:LYS:HE3	1:A:604:ASP:N	2.36	0.40
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.85	0.40

All (2) 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)
2:B:2:SER:OG	2:D:3:TYR:N[4_445]	1.31	0.89
1:A:101:GLN:OE1	1:A:603:LYS:NZ[3_545]	2.06	0.14

## 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	613/624 (98%)	566 (92%)	36 (6%)	11 (2%)	8	41
1	C	599/624 (96%)	561 (94%)	33 (6%)	5 (1%)	19	58
2	B	108/184 (59%)	89 (82%)	13 (12%)	6 (6%)	2	14
2	D	104/184 (56%)	90 (86%)	9 (9%)	5 (5%)	2	17
All	All	1424/1616 (88%)	1306 (92%)	91 (6%)	27 (2%)	8	39

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	7	LYS
1	A	317	CYS
1	A	384	THR
1	A	386	GLU
1	A	387	SER
1	A	526	PHE
2	B	55	ASP
2	B	64	VAL
2	B	127	SER
2	B	128	ILE
2	B	132	LYS
2	D	9	ASN
2	D	55	ASP
1	A	319	ASP
1	C	102	SER
2	D	23	LEU
2	D	105	ASN
1	A	320	GLU
2	B	23	LEU
1	C	317	CYS
2	D	131	GLU
1	C	105	ASP
1	C	536	ARG
1	C	551	TYR
1	A	388	PRO
1	A	391	GLY



### 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	558/564 (99%)	549 (98%)	9 (2%)	62	84
1	C	550/564 (98%)	540 (98%)	10 (2%)	59	82
2	B	99/161 (62%)	93 (94%)	6 (6%)	18	54
2	D	97/161 (60%)	94 (97%)	3 (3%)	40	72
3	E	2/4 (50%)	1 (50%)	1 (50%)	0	0
3	H	2/4 (50%)	1 (50%)	1 (50%)	0	0
All	All	1308/1458 (90%)	1278 (98%)	30 (2%)	50	78

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	144	TYR
1	A	181	PHE
1	A	204	ASN
1	A	259	PHE
1	A	320	GLU
1	A	389	LYS
1	A	621	SER
1	A	622	VAL
2	B	2	SER
2	B	7	ASP
2	B	61	ASN
2	B	64	VAL
2	B	67	THR
2	B	82	GLU
1	C	136	ARG
1	C	150	ASP
1	C	176	ARG
1	C	181	PHE
1	C	204	ASN
1	C	259	PHE
1	C	292	LEU

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Mol	Chain	Res	Type
1	C	398	ARG
1	C	475	ASP
1	C	536	ARG
2	D	37	ASN
2	D	63	ASN
2	D	105	ASN
3	E	3	PHE
3	H	6	ASP

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

Mol	Chain	Res	Type
2	B	121	HIS
2	B	125	ASN
1	C	208	ASN
2	D	37	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	TPO	H	4	3	8,10,11	1.91	3 (37%)	10,14,16	1.58	1 (10%)
3	TPO	E	4	3	8,10,11	2.08	2 (25%)	10,14,16	1.79	1 (10%)
3	SEP	E	5	3	8,9,10	1.76	2 (25%)	8,12,14	1.80	1 (12%)
3	SEP	H	5	3	8,9,10	1.70	1 (12%)	8,12,14	1.82	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPO	H	4	3	-	1/9/11/13	-
3	TPO	E	4	3	-	4/9/11/13	-
3	SEP	E	5	3	-	3/5/8/10	-
3	SEP	H	5	3	-	4/5/8/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	TPO	P-O1P	3.73	1.62	1.50
3	E	5	SEP	P-O1P	3.68	1.62	1.50
3	H	4	TPO	P-O1P	3.67	1.62	1.50
3	H	5	SEP	P-O1P	3.55	1.62	1.50
3	E	4	TPO	CB-CA	3.00	1.60	1.53
3	H	4	TPO	P-OG1	2.19	1.63	1.59
3	H	4	TPO	P-O2P	2.10	1.62	1.54
3	E	5	SEP	P-O2P	2.01	1.62	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	TPO	P-OG1-CB	-5.22	107.44	123.21
3	E	5	SEP	OG-CB-CA	4.41	112.43	108.14
3	H	4	TPO	P-OG1-CB	-4.29	110.26	123.21
3	H	5	SEP	OG-CB-CA	4.03	112.07	108.14
3	H	5	SEP	P-OG-CB	-2.25	112.11	118.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	4	TPO	CB-OG1-P-O1P
3	E	4	TPO	N-CA-CB-CG2
3	E	4	TPO	N-CA-CB-OG1
3	E	4	TPO	C-CA-CB-CG2
3	H	5	SEP	CB-OG-P-O3P
3	H	5	SEP	CB-OG-P-O1P
3	E	4	TPO	CB-OG1-P-O1P

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Mol	Chain	Res	Type	Atoms
3	E	5	SEP	CB-OG-P-O2P
3	H	5	SEP	CB-OG-P-O2P
3	E	5	SEP	CA-CB-OG-P
3	E	5	SEP	N-CA-CB-OG
3	H	5	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	TPO	1	0
3	E	5	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 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	617/624 (98%)	-0.19	6 (0%)	82 72	67, 101, 151, 191	0
1	C	605/624 (96%)	-0.04	6 (0%)	82 72	90, 125, 161, 182	0
2	B	114/184 (61%)	0.17	5 (4%)	34 21	80, 107, 148, 165	0
2	D	110/184 (59%)	0.69	14 (12%)	3 2	95, 142, 171, 180	0
3	E	2/6 (33%)	3.68	2 (100%)	0 0	182, 182, 182, 183	0
3	H	2/6 (33%)	0.24	0	100 100	170, 170, 170, 177	0
All	All	1450/1628 (89%)	-0.02	33 (2%)	60 47	67, 116, 161, 191	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	6	ASP	4.5
1	C	231	PRO	3.9
1	A	449	SER	3.8
2	D	7	ASP	3.8
1	A	451	ASP	3.6
1	C	272	THR	3.4
2	B	38	ALA	3.3
1	A	450	GLY	3.2
2	D	4	PRO	3.1
2	D	110	LEU	3.1
3	E	3	PHE	2.9
2	D	125	ASN	2.8
2	B	133	LYS	2.7
2	D	124	LEU	2.7
2	B	82	GLU	2.7
2	D	3	TYR	2.7
2	D	128	ILE	2.6
2	D	104	THR	2.6
1	A	452	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	388	PRO	2.4
2	B	31	GLY	2.4
1	A	387	SER	2.3
2	D	134	SER	2.3
2	D	106	PHE	2.3
2	D	101	TYR	2.2
1	C	270	LEU	2.2
1	C	451	ASP	2.2
2	B	105	ASN	2.1
2	D	130	ILE	2.1
2	D	31	GLY	2.0
1	C	411	GLY	2.0
2	D	92	PHE	2.0
1	C	414	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
3	TPO	E	4	11/12	0.65	0.58	194,208,242,254	0
3	SEP	E	5	10/11	0.73	0.44	189,200,212,225	0
3	SEP	H	5	10/11	0.77	0.26	176,197,209,213	0
3	TPO	H	4	11/12	0.85	0.41	183,196,215,229	0

## 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.