



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:17 AM GMT

PDB ID : 3HUF  
Title : Structure of the *S. pombe* Nbs1-Ctp1 complex  
Authors : Williams, R.S.; Guenther, G.; Tainer, J.A.  
Deposited on : 2009-06-13  
Resolution : 2.15 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

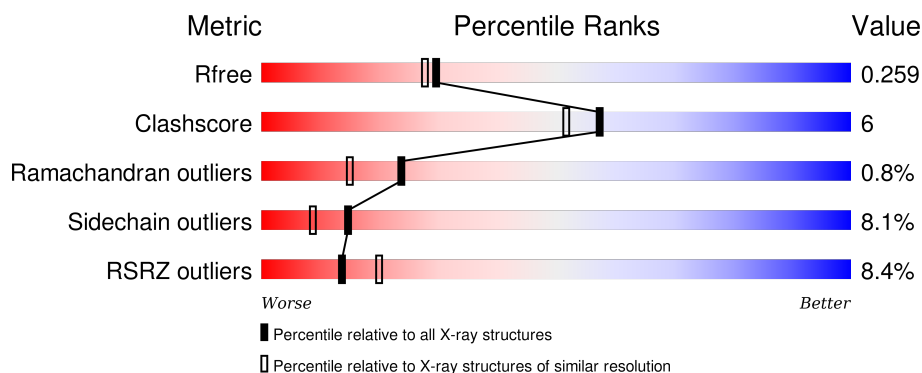
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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	325	<div> <div>8%</div> <div>76%</div> <div>15%</div> <div>7%</div> </div>
1	B	325	<div> <div>6%</div> <div>82%</div> <div>12%</div> <div>• •</div> </div>
1	C	325	<div> <div>10%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
2	E	13	<div> <div>8%</div> <div>38%</div> <div>62%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7688 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 DNA repair and telomere maintenance protein nbs1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2308	1467	381	445	15			
1	B	315	Total	C	N	O	S	0	0	0
			2461	1565	407	474	15			
1	C	313	Total	C	N	O	S	0	0	0
			2445	1552	406	472	15			

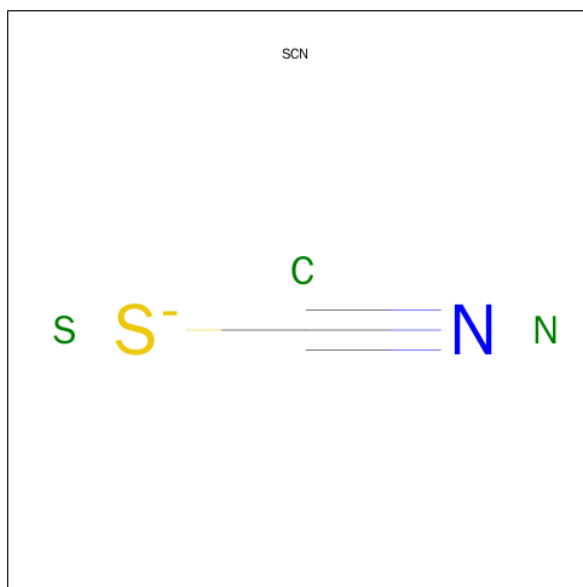
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	LEU	-	EXPRESSION TAG	UNP O43070
A	323	VAL	-	EXPRESSION TAG	UNP O43070
A	324	PRO	-	EXPRESSION TAG	UNP O43070
A	325	ARG	-	EXPRESSION TAG	UNP O43070
B	322	LEU	-	EXPRESSION TAG	UNP O43070
B	323	VAL	-	EXPRESSION TAG	UNP O43070
B	324	PRO	-	EXPRESSION TAG	UNP O43070
B	325	ARG	-	EXPRESSION TAG	UNP O43070
C	322	LEU	-	EXPRESSION TAG	UNP O43070
C	323	VAL	-	EXPRESSION TAG	UNP O43070
C	324	PRO	-	EXPRESSION TAG	UNP O43070
C	325	ARG	-	EXPRESSION TAG	UNP O43070

- Molecule 2 is a protein called Double-strand break repair protein ctp1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	P	0	0	0
			40	20	5	14	1			

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		

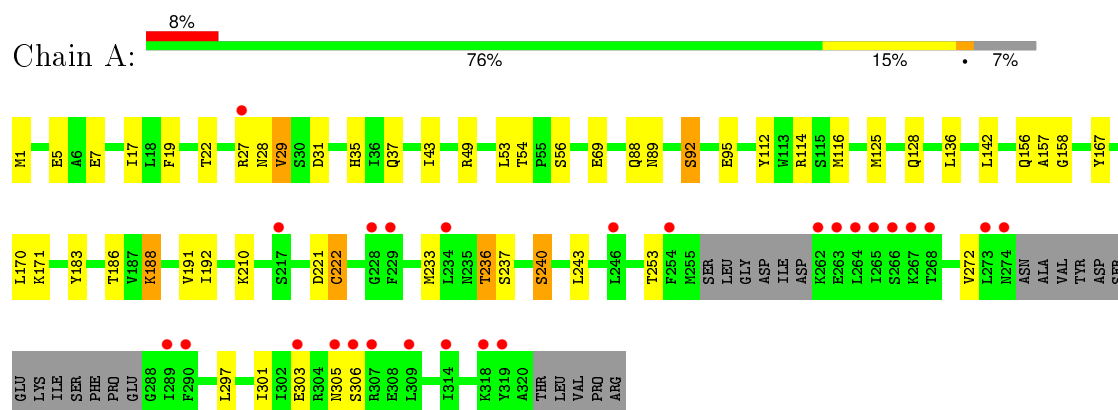
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	155	Total	O	0	0
			155	155		
4	C	129	Total	O	0	0
			129	129		
4	E	1	Total	O	0	0
			1	1		

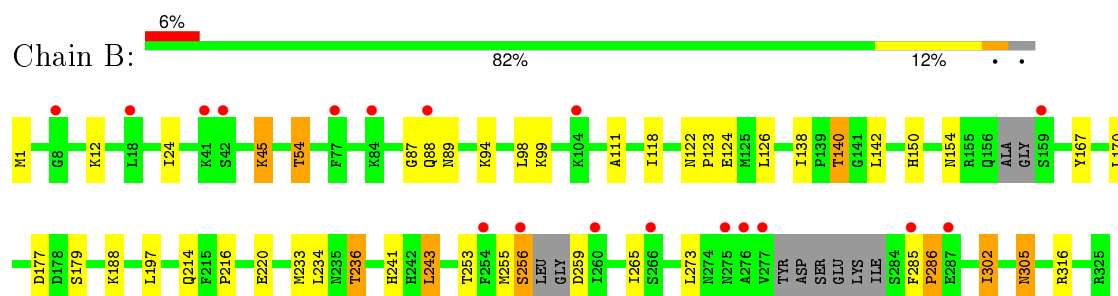
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

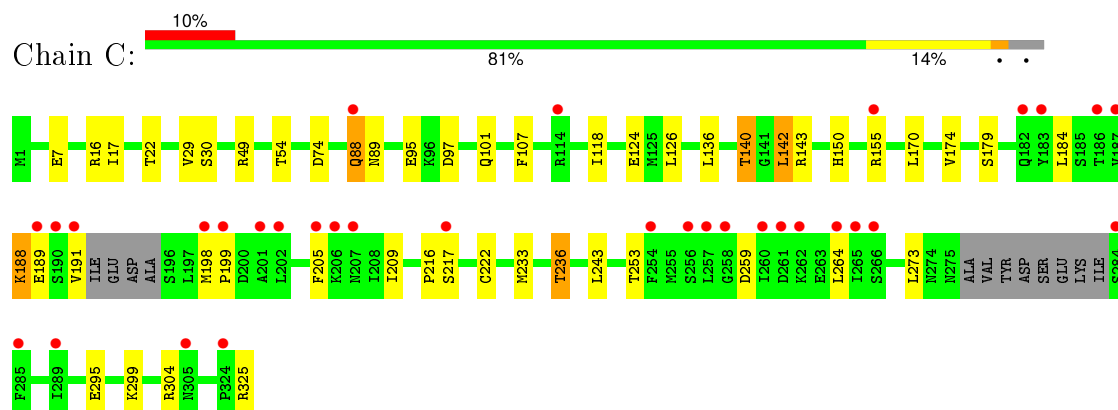
- Molecule 1: DNA repair and telomere maintenance protein nbs1



- Molecule 1: DNA repair and telomere maintenance protein nbs1

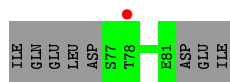


- Molecule 1: DNA repair and telomere maintenance protein nbs1



- Molecule 2: Double-strand break repair protein ctp1

Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.43 Å   244.63 Å   51.99 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.15 43.72 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (50.00-2.15) 97.0 (43.72-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.16 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.215   ,   0.262 0.214   ,   0.259	Depositor DCC
$R_{free}$ test set	3374 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 66605 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TPO, SCN, 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	0.57	0/2349	0.70	0/3177
1	B	0.55	0/2503	0.67	1/3379 (0.0%)
1	C	0.55	0/2488	0.67	0/3360
2	E	0.77	0/22	0.69	0/27
All	All	0.56	0/7362	0.68	1/9943 (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	B	286	PRO	N-CA-CB	6.16	110.69	103.30

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	2308	0	2241	27	0
1	B	2461	0	2435	32	0
1	C	2445	0	2417	27	0
2	E	40	0	26	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	143	0	0	2	0
4	B	155	0	0	6	0
4	C	129	0	0	5	0
4	E	1	0	0	0	0
All	All	7688	0	7119	86	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 6.

All (86) 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:B:126:LEU:HD11	1:B:140:THR:HG23	1.62	0.82
1:B:256:SER:HG	1:B:259:ASP:N	1.79	0.81
1:A:233:MET:HG3	1:A:236:THR:HG22	1.64	0.79
1:B:243:LEU:HD12	1:B:243:LEU:C	2.04	0.78
1:C:198:MET:HB2	1:C:199:PRO:HD2	1.66	0.76
1:C:17:ILE:H	1:C:191:VAL:HG11	1.51	0.75
1:A:29:VAL:HG13	1:A:35:HIS:HB3	1.72	0.69
1:C:295:GLU:O	1:C:299:LYS:HD3	1.94	0.69
1:A:69:GLU:HG2	1:A:92:SER:HB3	1.75	0.67
1:C:7:GLU:HG2	1:C:107:PHE:HD2	1.60	0.67
1:B:45:LYS:NZ	1:B:45:LYS:HB3	2.11	0.66
1:C:7:GLU:HG2	1:C:107:PHE:CD2	2.31	0.66
1:A:1:MET:HE2	1:A:17:ILE:CG2	2.26	0.66
1:B:140:THR:HG22	4:B:376:HOH:O	1.98	0.63
1:C:170:LEU:HD12	1:C:243:LEU:HD13	1.81	0.62
1:C:88:GLN:O	1:C:89:ASN:HB2	1.99	0.62
1:B:236:THR:HG23	1:B:253:THR:HG23	1.82	0.61
1:A:233:MET:HG3	1:A:236:THR:CG2	2.31	0.61
1:C:299:LYS:HD2	4:C:446:HOH:O	2.00	0.61
1:B:305:ASN:H	1:B:305:ASN:ND2	1.99	0.60
1:B:305:ASN:HD22	1:B:305:ASN:H	1.50	0.59
1:C:22:THR:HG21	1:C:49:ARG:NH1	2.17	0.59
1:B:243:LEU:HD12	1:B:243:LEU:O	2.03	0.58
1:A:156:GLN:O	1:A:158:GLY:N	2.35	0.58
1:B:45:LYS:HZ2	1:B:45:LYS:HB3	1.69	0.57
1:A:237:SER:HG	1:A:240:SER:HG	1.52	0.57
1:B:54:THR:HG23	4:B:412:HOH:O	2.05	0.57
1:C:136:LEU:HD21	1:C:188:LYS:HD2	1.89	0.54
1:A:27:ARG:NH1	1:A:43:ILE:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TYR:O	1:A:186:THR:HB	2.09	0.53
1:A:1:MET:HE1	1:A:19:PHE:CE2	2.44	0.53
1:C:7:GLU:CD	4:C:366:HOH:O	2.47	0.52
1:A:170:LEU:HD21	1:A:222:CYS:HB3	1.90	0.52
1:B:243:LEU:C	1:B:243:LEU:CD1	2.78	0.52
1:B:170:LEU:CD1	1:B:243:LEU:HD13	2.40	0.52
1:B:98:LEU:HB2	1:B:111:ALA:HB3	1.92	0.51
1:C:17:ILE:H	1:C:191:VAL:CG1	2.23	0.51
1:C:126:LEU:HD22	1:C:142:LEU:HD23	1.92	0.50
1:A:29:VAL:O	1:A:37:GLN:HB2	2.12	0.50
1:C:304:ARG:NH2	4:C:454:HOH:O	2.20	0.49
1:A:1:MET:HE2	1:A:17:ILE:HG23	1.94	0.49
1:B:233:MET:SD	1:B:236:THR:HB	2.52	0.49
1:A:136:LEU:HD23	1:A:188:LYS:HG2	1.94	0.49
1:B:177:ASP:OD2	1:B:179:SER:OG	2.26	0.49
1:C:236:THR:HG23	1:C:253:THR:OG1	2.13	0.48
1:C:101:GLN:NE2	4:C:390:HOH:O	2.46	0.48
1:C:205:PHE:CE1	1:C:209:ILE:HD11	2.48	0.48
1:A:22:THR:HG21	1:A:49:ARG:HD3	1.96	0.47
1:A:233:MET:HB3	1:A:272:VAL:O	2.15	0.47
1:A:116:MET:N	4:A:386:HOH:O	2.47	0.47
1:C:118:ILE:HG12	1:C:150:HIS:HB2	1.97	0.47
1:C:216:PRO:HG3	1:C:222:CYS:SG	2.55	0.47
1:A:1:MET:CE	1:A:17:ILE:CG2	2.92	0.46
1:B:87:GLY:O	4:B:428:HOH:O	2.20	0.46
1:B:1:MET:CE	1:B:197:LEU:HD12	2.46	0.46
1:C:233:MET:SD	1:C:236:THR:HB	2.56	0.46
1:A:236:THR:HG23	1:A:253:THR:HG23	1.98	0.46
1:A:53:LEU:HG	4:A:388:HOH:O	2.15	0.46
1:A:5:GLU:HG2	1:A:112:TYR:HE2	1.81	0.45
1:A:17:ILE:HD12	1:A:192:ILE:HG13	1.98	0.44
1:C:236:THR:HG23	1:C:253:THR:HG23	2.00	0.44
1:A:167:TYR:O	1:A:171:LYS:HG2	2.17	0.44
1:A:1:MET:HE1	1:A:19:PHE:CD2	2.53	0.44
1:C:205:PHE:CZ	1:C:209:ILE:HD11	2.53	0.44
1:B:122:ASN:OD1	1:B:124:GLU:HG2	2.18	0.43
1:A:88:GLN:O	1:A:89:ASN:HB2	2.18	0.43
1:B:54:THR:HG22	4:B:348:HOH:O	2.17	0.43
1:C:17:ILE:N	1:C:191:VAL:HG11	2.28	0.43
1:A:1:MET:N	1:A:114:ARG:O	2.52	0.43
1:B:236:THR:HG23	1:B:253:THR:CG2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:HIS:HE1	4:B:451:HOH:O	2.01	0.42
1:B:122:ASN:HA	1:B:123:PRO:HD3	1.83	0.42
1:B:123:PRO:HG3	1:B:142:LEU:HD21	2.01	0.42
1:A:88:GLN:H	1:A:88:GLN:HG2	1.67	0.42
1:B:140:THR:CG2	4:B:376:HOH:O	2.63	0.42
1:B:167:TYR:CD1	1:B:243:LEU:HB2	2.55	0.42
1:C:304:ARG:NE	4:C:454:HOH:O	2.47	0.42
1:C:236:THR:HG23	1:C:253:THR:CG2	2.50	0.42
1:B:216:PRO:HD3	1:B:302:ILE:HD11	2.03	0.41
1:B:1:MET:HE3	1:B:197:LEU:HD12	2.02	0.41
1:B:118:ILE:HG12	1:B:150:HIS:HB2	2.02	0.41
1:B:305:ASN:HD22	1:B:305:ASN:N	2.19	0.40
1:B:118:ILE:HD12	1:B:138:ILE:HG21	2.02	0.40
1:C:126:LEU:HD11	1:C:140:THR:HG23	2.03	0.40
1:C:174:VAL:HG13	1:C:205:PHE:HB2	2.03	0.40
1:B:265:ILE:HD13	1:B:265:ILE:HA	1.92	0.40

There are no symmetry-related clashes.

## 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	295/325 (91%)	277 (94%)	13 (4%)	5 (2%)	11	4
1	B	307/325 (94%)	300 (98%)	5 (2%)	2 (1%)	26	18
1	C	307/325 (94%)	297 (97%)	10 (3%)	0	100	100
2	E	2/13 (15%)	1 (50%)	1 (50%)	0	100	100
All	All	911/988 (92%)	875 (96%)	29 (3%)	7 (1%)	24	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	GLU
1	B	285	PHE
1	B	286	PRO
1	A	31	ASP
1	A	306	SER
1	A	157	ALA
1	A	305	ASN

### 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	252/295 (85%)	232 (92%)	20 (8%)	15	9
1	B	276/295 (94%)	254 (92%)	22 (8%)	15	9
1	C	275/295 (93%)	252 (92%)	23 (8%)	14	8
2	E	3/11 (27%)	3 (100%)	0	100	100
All	All	806/896 (90%)	741 (92%)	65 (8%)	15	9

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	28	ASN
1	A	29	VAL
1	A	54	THR
1	A	56	SER
1	A	92	SER
1	A	95	GLU
1	A	125	MET
1	A	128	GLN
1	A	142	LEU
1	A	188	LYS
1	A	191	VAL
1	A	210	LYS
1	A	221	ASP
1	A	222	CYS

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Mol	Chain	Res	Type
1	A	236	THR
1	A	240	SER
1	A	243	LEU
1	A	297	LEU
1	A	301	ILE
1	B	12	LYS
1	B	24	ILE
1	B	45	LYS
1	B	54	THR
1	B	88	GLN
1	B	89	ASN
1	B	94	LYS
1	B	99	LYS
1	B	140	THR
1	B	154	ASN
1	B	188	LYS
1	B	214	GLN
1	B	220	GLU
1	B	234	LEU
1	B	236	THR
1	B	243	LEU
1	B	255	MET
1	B	256	SER
1	B	273	LEU
1	B	302	ILE
1	B	305	ASN
1	B	316	ARG
1	C	16	ARG
1	C	29	VAL
1	C	30	SER
1	C	54	THR
1	C	74	ASP
1	C	88	GLN
1	C	95	GLU
1	C	97	ASP
1	C	124	GLU
1	C	140	THR
1	C	142	LEU
1	C	143	ARG
1	C	155	ARG
1	C	179	SER
1	C	184	LEU

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Mol	Chain	Res	Type
1	C	188	LYS
1	C	189	GLU
1	C	217	SER
1	C	236	THR
1	C	259	ASP
1	C	264	LEU
1	C	273	LEU
1	C	325	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	B	28	ASN
1	B	134	ASN
1	B	154	ASN
1	B	242	HIS
1	B	305	ASN
1	C	89	ASN
1	C	132	ASN
1	C	134	ASN
1	C	156	GLN
1	C	275	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
2	SEP	E	77	2	3,4,10	0.59	0	0,4,14	0.00	-
2	TPO	E	79	2	8,10,11	0.57	0	7,14,16	1.30	1 (14%)

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
2	SEP	E	77	2	-	0/0/2/10	0/0/0/0
2	TPO	E	79	2	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	79	TPO	O-C-CA	-2.11	119.86	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SCN	A	326	-	2,2,2	1.43	0	1,1,1	1.60	0
3	SCN	B	326	-	2,2,2	1.11	0	1,1,1	1.73	0

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	SCN	A	326	-	-	0/0/0/0	0/0/0/0
3	SCN	B	326	-	-	0/0/0/0	0/0/0/0

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 [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	301/325 (92%)	0.60	26 (8%) 13 19	32, 43, 66, 76	0
1	B	315/325 (96%)	0.46	18 (5%) 27 37	28, 42, 62, 76	0
1	C	313/325 (96%)	0.66	33 (10%) 8 13	30, 41, 70, 84	0
2	E	3/13 (23%)	1.99	1 (33%) 0 1	58, 58, 60, 60	0
All	All	932/988 (94%)	0.57	78 (8%) 14 20	28, 42, 66, 84	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	ARG	7.9
1	A	306	SER	7.8
1	C	186	THR	6.8
1	A	265	ILE	6.6
1	C	257	LEU	6.4
1	C	284	SER	6.3
1	A	305	ASN	5.5
1	A	309	LEU	5.5
1	A	254	PHE	5.4
1	C	266	SER	5.2
1	B	77	PHE	4.7
1	A	266	SER	4.6
1	B	88	GLN	4.5
1	A	264	LEU	4.1
1	A	289	ILE	4.1
1	C	191	VAL	4.1
1	B	285	PHE	4.1
1	A	314	ILE	4.0
1	C	264	LEU	3.9
1	B	277	VAL	3.9
1	A	273	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	183	TYR	3.7
1	C	260	ILE	3.7
1	C	182	GLN	3.6
1	A	268	THR	3.6
1	C	201	ALA	3.6
1	B	260	ILE	3.5
1	C	258	GLY	3.5
1	B	8	GLY	3.4
1	A	234	LEU	3.4
1	A	228	GLY	3.4
1	B	84	LYS	3.3
1	A	267	LYS	3.3
1	C	261	ASP	3.2
1	B	256	SER	3.1
1	B	41	LYS	3.1
1	C	198	MET	3.1
1	C	262	LYS	3.0
1	A	263	GLU	2.9
1	A	217	SER	2.9
1	C	187	VAL	2.9
1	C	189	GLU	2.8
1	A	274	ASN	2.8
1	C	202	LEU	2.8
1	C	207	ASN	2.8
1	B	276	ALA	2.8
1	A	262	LYS	2.7
1	A	290	PHE	2.7
1	C	190	SER	2.6
1	A	319	TYR	2.6
2	E	78	THR	2.6
1	A	27	ARG	2.5
1	A	246	LEU	2.5
1	B	287	GLU	2.5
1	B	159	SER	2.5
1	A	303	GLU	2.4
1	C	114	ARG	2.4
1	A	229	PHE	2.4
1	C	289	ILE	2.3
1	C	285	PHE	2.3
1	B	42	SER	2.3
1	C	305	ASN	2.3
1	C	265	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	18	LEU	2.3
1	C	199	PRO	2.3
1	C	254	PHE	2.2
1	A	318	LYS	2.2
1	C	217	SER	2.2
1	B	275	ASN	2.2
1	B	266	SER	2.2
1	B	104	LYS	2.1
1	C	155	ARG	2.1
1	C	324	PRO	2.1
1	B	254	PHE	2.1
1	C	205	PHE	2.0
1	C	256	SER	2.0
1	C	88	GLN	2.0
1	C	206	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	TPO	E	79	11/12	0.71	0.21	-	58,59,60,61	0
2	SEP	E	77	5/11	0.84	0.29	-	59,59,59,59	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SCN	A	326	3/3	0.98	0.10	-1.67	28,28,28,29	0
3	SCN	B	326	3/3	0.96	0.09	-2.49	28,28,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.