



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 05:17 AM EDT

PDB ID : 5HB3  
Title : Crystal structure of Chaetomium thermophilum Nic96 SOL-Nup53 complex  
Authors : Lin, D.H.; Stuwe, T.; Hoelz, A.  
Deposited on : unknown  
Resolution : 2.65 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

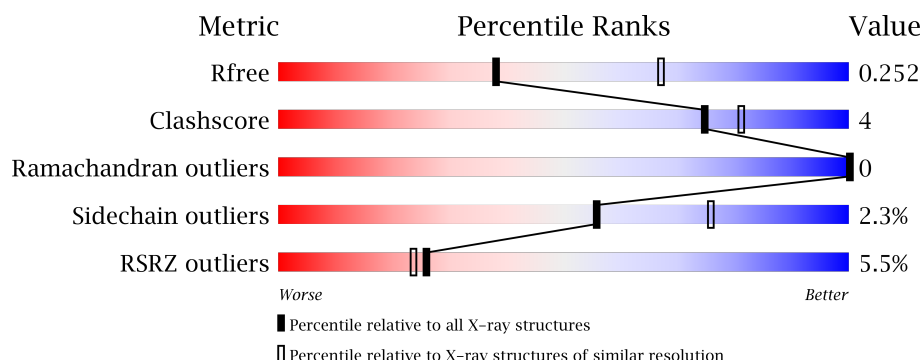
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	723	<div> <div>7%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	C	723	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
2	B	55	<div> <div>5%</div> <div>27%</div> <div>..</div> <div>67%</div> </div>
2	D	55	<div> <div>2%</div> <div>22%</div> <div>9%</div> <div>69%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23000 atoms, of which 11431 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 Nucleoporin NIC96.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	703	Total	C	H	N	O	S	0	1	0
			11153	3520	5564	999	1036	34			
1	C	709	Total	C	H	N	O	S	0	1	0
			11250	3549	5610	1011	1047	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	390	SER	-	expression tag	UNP G0S024
C	390	SER	-	expression tag	UNP G0S024

- Molecule 2 is a protein called Nucleoporin NUP53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	H	N	O	0	0	0
			267	88	130	22	27			
2	D	17	Total	C	H	N	O	0	0	0
			256	84	127	21	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	SER	-	expression tag	UNP G0S156
D	30	SER	-	expression tag	UNP G0S156

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	2	Total	Cl	0	0
			2	2		

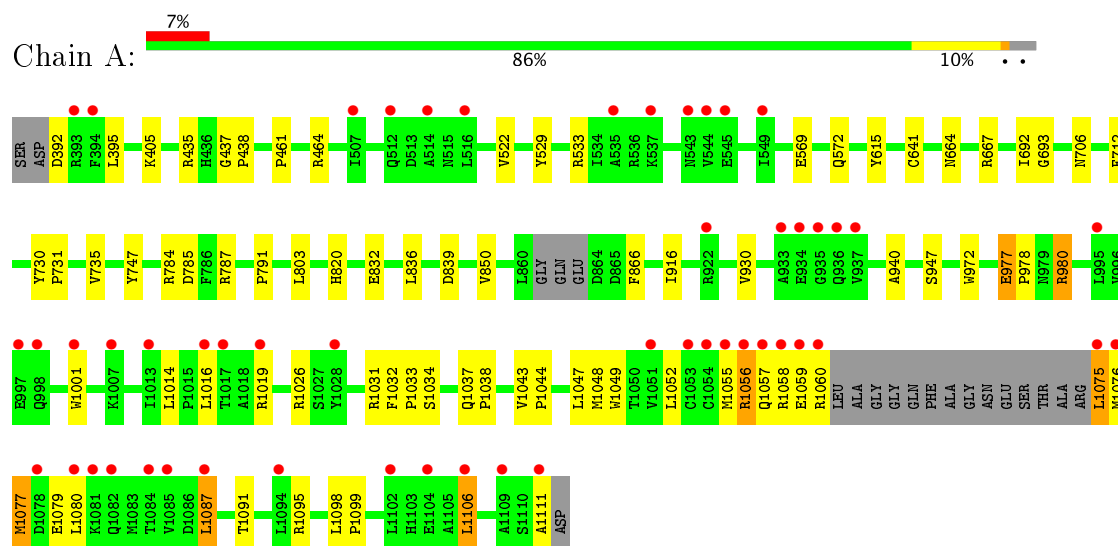
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0
4	C	35	Total 35	O 35	0	0

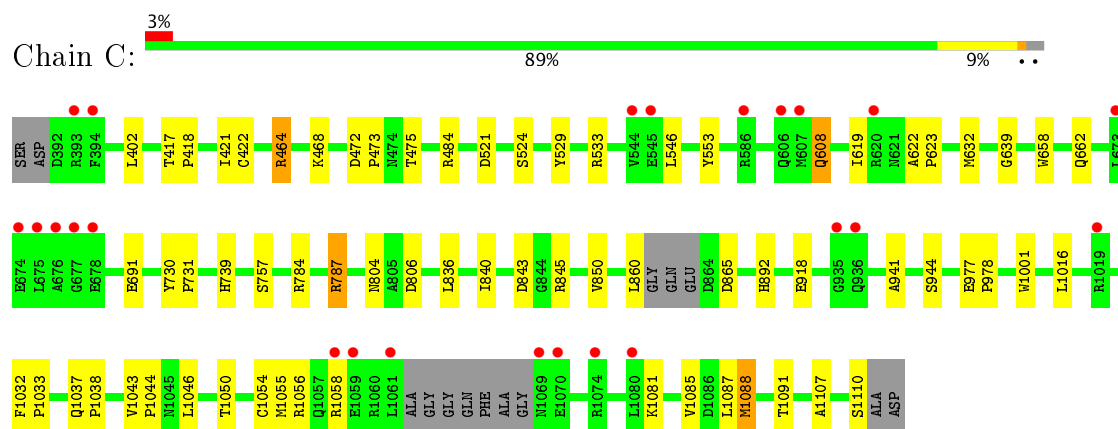
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

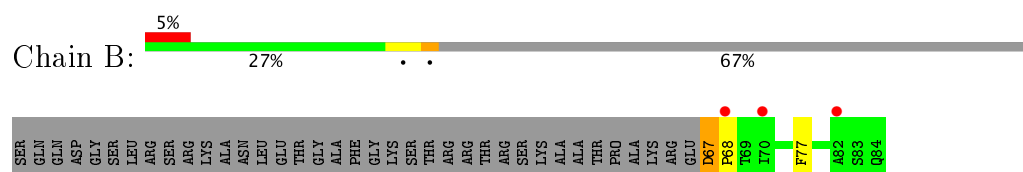
#### • Molecule 1: Nucleoporin NIC96



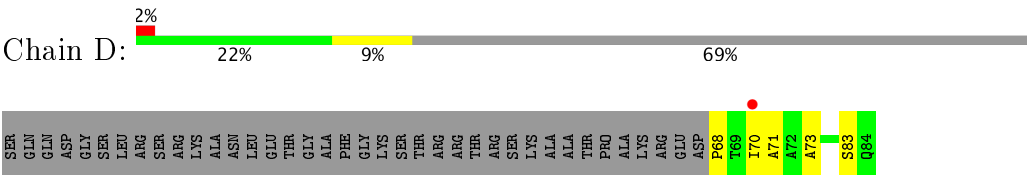
#### • Molecule 1: Nucleoporin NIC96



#### • Molecule 2: Nucleoporin NUP53



● Molecule 2: Nucleoporin NUP53



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.52Å 86.95Å 98.01Å 100.69° 99.59° 95.66°	Depositor
Resolution (Å)	47.28 – 2.65 47.29 – 2.65	Depositor EDS
% Data completeness (in resolution range)	88.5 (47.28-2.65) 83.0 (47.29-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.212 , 0.249 0.215 , 0.252	Depositor DCC
$R_{free}$ test set	2368 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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:  
CL

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	0.22	0/5696	0.38	0/7702
1	C	0.22	0/5748	0.37	0/7773
2	B	0.20	0/140	0.32	0/191
2	D	0.20	0/132	0.34	0/179
All	All	0.22	0/11716	0.38	0/15845

There are no bond length outliers.

There are no bond angle outliers.

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	5589	5564	5549	44	0
1	C	5640	5610	5595	37	0
2	B	137	130	130	2	0
2	D	129	127	127	3	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
4	A	36	0	0	0	0
4	C	35	0	0	0	0
All	All	11569	11431	11401	85	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 4.

All (85) 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:C:1081:LYS:O	1:C:1085:VAL:HG23	2.03	0.58
1:C:622:ALA:HB1	1:C:623:PRO:CD	2.36	0.55
1:C:622:ALA:HB1	1:C:623:PRO:HD2	1.90	0.54
2:D:68:PRO:HA	2:D:71:ALA:HB3	1.90	0.53
1:C:1037:GLN:HB3	1:C:1038:PRO:HD3	1.90	0.53
1:C:1001:TRP:CZ2	1:C:1056:ARG:HG2	2.44	0.53
1:C:1050:THR:O	1:C:1054:CYS:HB2	2.10	0.52
1:A:692:ILE:HD13	2:B:77:PHE:CE2	2.45	0.52
1:C:1043:VAL:N	1:C:1044:PRO:CD	2.72	0.52
1:A:839:ASP:OD2	1:A:947:SER:HB3	2.10	0.52
1:C:840:ILE:HD13	1:C:892:HIS:CD2	2.46	0.51
1:A:1057:GLN:CG	1:A:1080:LEU:HD13	2.41	0.51
1:A:1032:PHE:N	1:A:1033:PRO:HD2	2.25	0.51
1:C:1055:MET:SD	1:C:1110:SER:HA	2.51	0.51
1:A:972:TRP:CZ2	1:A:980:ARG:HD3	2.45	0.50
1:A:1014:LEU:HB2	1:A:1016:LEU:HD13	1.93	0.50
1:A:1043:VAL:N	1:A:1044:PRO:CD	2.75	0.50
1:A:1016:LEU:HD11	1:A:1087:LEU:HD11	1.93	0.49
1:A:569:GLU:HA	1:A:572:GLN:HG2	1.93	0.49
1:C:843:ASP:OD2	1:C:845:ARG:NE	2.45	0.49
1:C:464:ARG:NH2	1:C:804:ASN:OD1	2.46	0.49
1:A:1048:MET:SD	1:A:1106:LEU:HD12	2.53	0.48
1:A:1075:LEU:C	1:A:1075:LEU:HD22	2.34	0.48
1:C:546:LEU:HB2	1:C:553:TYR:CD1	2.48	0.48
1:A:1052:LEU:O	1:A:1056:ARG:HG2	2.13	0.48
1:C:1032:PHE:HB3	1:C:1033:PRO:HD3	1.96	0.48
1:C:529:TYR:CZ	1:C:533:ARG:HD2	2.49	0.48
1:C:977:GLU:N	1:C:978:PRO:HD2	2.29	0.47
1:C:1046:LEU:O	1:C:1050:THR:HG23	2.14	0.47
2:D:83:SER:O	2:D:83:SER:OG	2.29	0.47
1:C:475:THR:O	1:C:484:ARG:NH2	2.48	0.47
1:C:521:ASP:OD1	1:C:524:SER:OG	2.23	0.46
1:A:916:ILE:HD11	1:A:1049:TRP:NE1	2.31	0.46
1:A:1075:LEU:O	1:A:1075:LEU:HD22	2.15	0.46
1:A:464:ARG:HD2	1:A:803:LEU:O	2.15	0.46
1:A:1019:ARG:NE	1:A:1079:GLU:OE1	2.48	0.46
1:C:784:ARG:HA	1:C:787:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:ILE:HA	2:D:73:ALA:HB3	1.97	0.46
1:C:608:GLN:NE2	1:C:639:GLY:O	2.47	0.45
1:A:1077:MET:SD	1:A:1077:MET:N	2.89	0.45
1:A:615:TYR:CD2	1:A:641:CYS:HB3	2.51	0.45
1:A:839:ASP:OD2	1:A:947:SER:CB	2.64	0.45
1:A:977:GLU:N	1:A:978:PRO:HD2	2.31	0.45
1:A:1055:MET:HE2	1:A:1111:ALA:HB2	1.98	0.45
1:C:730:TYR:HB3	1:C:731:PRO:HD3	1.98	0.45
1:C:1016:LEU:N	1:C:1016:LEU:HD12	2.32	0.45
1:A:529:TYR:OH	1:A:533:ARG:NH1	2.49	0.44
1:C:1088:MET:CE	1:C:1107:ALA:HB2	2.47	0.44
1:A:730:TYR:N	1:A:731:PRO:CD	2.80	0.44
1:C:417:THR:HG23	1:C:418:PRO:HD2	1.99	0.44
1:C:464:ARG:HD3	1:C:806:ASP:OD2	2.16	0.44
1:C:836:LEU:HA	1:C:850:VAL:HG12	1.98	0.44
1:C:619:ILE:CG2	1:C:632:MET:HG2	2.47	0.44
1:A:461:PRO:HG2	1:A:747:TYR:CE1	2.53	0.44
1:A:784:ARG:HG2	1:A:787:ARG:HD3	1.99	0.44
1:C:941:ALA:O	1:C:944:SER:OG	2.21	0.44
1:A:1037:GLN:N	1:A:1038:PRO:HD2	2.33	0.43
1:A:1056:ARG:O	1:A:1059:GLU:HB3	2.18	0.43
1:A:437:GLY:N	1:A:438:PRO:HD2	2.33	0.43
1:A:930:VAL:HG21	1:A:940:ALA:HB3	1.99	0.43
1:A:1047:LEU:CD1	1:A:1091:THR:HG22	2.49	0.43
1:C:1055:MET:O	1:C:1058:ARG:HG2	2.19	0.43
1:A:395:LEU:HD11	1:A:735:VAL:HG21	2.01	0.42
1:A:1043:VAL:N	1:A:1044:PRO:HD2	2.34	0.42
1:A:836:LEU:HA	1:A:850:VAL:HG12	2.01	0.42
1:C:402:LEU:HD13	1:C:739:HIS:CE1	2.54	0.42
1:A:1031:ARG:O	1:A:1034:SER:OG	2.27	0.42
1:C:1087:LEU:O	1:C:1091:THR:HG23	2.20	0.42
1:C:1043:VAL:N	1:C:1044:PRO:HD2	2.34	0.42
1:A:522:VAL:HG21	1:A:569:GLU:HG2	2.01	0.42
2:B:67:ASP:N	2:B:68:PRO:CD	2.82	0.42
1:C:472:ASP:HA	1:C:473:PRO:HD3	1.95	0.41
1:C:464:ARG:CD	1:C:806:ASP:OD2	2.67	0.41
1:A:1001:TRP:HE1	1:A:1056:ARG:HG3	1.85	0.41
1:C:658:TRP:O	1:C:662:GLN:HG2	2.21	0.41
1:A:820:HIS:HB3	1:A:866:PHE:CE1	2.56	0.41
1:A:1098:LEU:HB3	1:A:1099:PRO:CD	2.50	0.41
1:A:1098:LEU:HB3	1:A:1099:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:TYR:N	1:C:731:PRO:CD	2.83	0.41
1:C:421:ILE:HG23	1:C:422:CYS:N	2.36	0.40
1:A:664:ASN:O	1:A:667:ARG:NH2	2.50	0.40
1:A:1001:TRP:CZ3	1:A:1060:ARG:NH1	2.90	0.40
1:A:693:GLY:HA3	1:A:712:PHE:CZ	2.57	0.40
1:A:1055:MET:CE	1:A:1111:ALA:HB2	2.52	0.40
1:A:791:PRO:HG2	1:A:832:GLU:HG3	2.03	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	698/723 (96%)	668 (96%)	30 (4%)	0	100	100
1	C	704/723 (97%)	678 (96%)	26 (4%)	0	100	100
2	B	16/55 (29%)	16 (100%)	0	0	100	100
2	D	15/55 (27%)	14 (93%)	1 (7%)	0	100	100
All	All	1433/1556 (92%)	1376 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	584/596 (98%)	568 (97%)	16 (3%)	50	71
1	C	590/596 (99%)	580 (98%)	10 (2%)	66	83
2	B	14/43 (33%)	13 (93%)	1 (7%)	17	27
2	D	13/43 (30%)	13 (100%)	0	100	100
All	All	1201/1278 (94%)	1174 (98%)	27 (2%)	56	77

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	ASP
1	A	405	LYS
1	A	435	ARG
1	A	706	ASN
1	A	785	ASP
1	A	977	GLU
1	A	980	ARG
1	A	1026	ARG
1	A	1056	ARG
1	A	1058	ARG
1	A	1075	LEU
1	A	1076	MET
1	A	1077	MET
1	A	1087	LEU
1	A	1095	ARG
1	A	1106	LEU
2	B	67	ASP
1	C	464	ARG
1	C	468	LYS
1	C	608	GLN
1	C	691	GLU
1	C	757	SER
1	C	787	ARG
1	C	860	LEU
1	C	865	ASP
1	C	918	GLU
1	C	1088	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	572	GLN

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Mol	Chain	Res	Type
1	A	716	GLN
1	A	760	ASN
1	A	1103	HIS
1	C	486	GLN
1	C	572	GLN
1	C	578	GLN
1	C	645	ASN
1	C	932	ASN

### 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 carbohydrates 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 ⓘ

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	703/723 (97%)	0.49	52 (7%) 15 13	32, 60, 109, 124	0
1	C	709/723 (98%)	0.32	24 (3%) 46 44	35, 56, 105, 130	0
2	B	18/55 (32%)	0.53	3 (16%) 2 1	66, 79, 91, 97	0
2	D	17/55 (30%)	0.59	1 (5%) 23 21	63, 79, 87, 87	0
All	All	1447/1556 (92%)	0.41	80 (5%) 26 24	32, 58, 106, 130	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	935	GLY	8.5
1	A	1060	ARG	8.3
1	A	1057	GLN	8.2
1	A	1087	LEU	7.2
1	C	676	ALA	7.1
1	A	1078	ASP	6.2
1	A	1080	LEU	6.2
1	C	673	LEU	6.1
1	A	1109	ALA	5.8
1	A	394	PHE	5.7
1	A	1051	VAL	5.5
1	A	1055	MET	5.4
1	C	677	GLY	5.3
1	A	936	GLN	5.0
1	C	1019	ARG	4.9
1	C	935	GLY	4.5
1	C	1059	GLU	4.3
1	A	934	GLU	4.3
1	C	675	LEU	4.2
1	A	512	GLN	4.2
1	C	1070	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1019	ARG	4.0
1	A	1104	GLU	3.8
2	D	70	ILE	3.8
1	C	606	GLN	3.6
1	A	1053	CYS	3.6
1	C	678	GLU	3.5
1	A	514	ALA	3.4
1	C	1074	ARG	3.4
1	A	1056	ARG	3.2
1	A	1016	LEU	3.2
1	A	1001	TRP	3.2
1	A	516	LEU	3.1
1	A	393	ARG	3.1
2	B	68	PRO	3.1
1	A	1081	LYS	3.1
1	A	1085	VAL	3.1
1	A	922	ARG	3.0
1	A	544	VAL	2.9
1	A	543	ASN	2.9
1	A	937	VAL	2.9
1	A	1054	CYS	2.9
1	C	1061	LEU	2.9
1	C	394	PHE	2.8
1	C	936	GLN	2.8
1	A	933	ALA	2.8
1	A	1059	GLU	2.7
1	A	1058	ARG	2.7
1	A	545	GLU	2.7
1	A	1102	LEU	2.7
1	C	1069	ASN	2.7
1	C	674	GLU	2.6
1	C	1080	LEU	2.6
2	B	82	ALA	2.6
1	C	393	ARG	2.6
1	A	995	LEU	2.5
1	A	507	ILE	2.4
1	A	998	GLN	2.4
1	A	535	ALA	2.4
2	B	70	ILE	2.4
1	A	1082	GLN	2.3
1	A	1075	LEU	2.3
1	A	1084	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1111	ALA	2.3
1	C	1058	ARG	2.3
1	A	1106	LEU	2.3
1	C	586	ARG	2.2
1	A	1007	LYS	2.2
1	C	545	GLU	2.2
1	A	1013	ILE	2.2
1	C	544	VAL	2.2
1	A	997	GLU	2.2
1	A	1017	THR	2.1
1	A	1094	LEU	2.1
1	A	1028	TYR	2.1
1	C	607	MET	2.1
1	C	620	ARG	2.1
1	A	549	ILE	2.0
1	A	537	LYS	2.0
1	A	1076	MET	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 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(Å <sup>2</sup> )	Q<0.9
3	CL	A	1201	1/1	0.91	0.14	-1.48	62,62,62,62	0
3	CL	C	1202	1/1	0.97	0.14	-2.80	51,51,51,51	0
3	CL	C	1201	1/1	0.94	0.13	-2.93	57,57,57,57	0

## 6.5 Other polymers

There are no such residues in this entry.