



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:01 PM GMT

PDB ID : 2DOQ  
Title : crystal structure of Sfi1p/Cdc31p complex  
Authors : Li, S.; Sandercock, A.M.; Conduit, P.T.; Robinson, C.V.; Williams, R.L.;  
Kilmartin, J.V.  
Deposited on : 2006-05-03  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

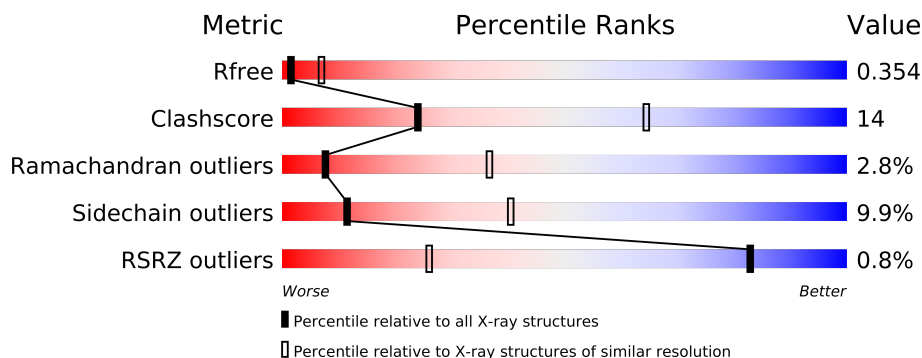
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	161	
1	B	161	
1	C	161	
2	D	94	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4230 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cell division control protein 31.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	Se	0	0	0
			1205	762	192	245	1	5			
1	B	149	Total	C	N	O	S	Se	0	0	0
			1227	775	196	250	1	5			
1	C	130	Total	C	N	O	S	Se	0	0	0
			1083	691	174	213	5				

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P06704
A	34	MSE	MET	MODIFIED RESIDUE	UNP P06704
A	49	MSE	MET	MODIFIED RESIDUE	UNP P06704
A	76	MSE	MET	MODIFIED RESIDUE	UNP P06704
A	85	MSE	MET	MODIFIED RESIDUE	UNP P06704
A	137	MSE	MET	MODIFIED RESIDUE	UNP P06704
B	1	MSE	MET	MODIFIED RESIDUE	UNP P06704
B	34	MSE	MET	MODIFIED RESIDUE	UNP P06704
B	49	MSE	MET	MODIFIED RESIDUE	UNP P06704
B	76	MSE	MET	MODIFIED RESIDUE	UNP P06704
B	85	MSE	MET	MODIFIED RESIDUE	UNP P06704
B	137	MSE	MET	MODIFIED RESIDUE	UNP P06704
C	1	MSE	MET	MODIFIED RESIDUE	UNP P06704
C	34	MSE	MET	MODIFIED RESIDUE	UNP P06704
C	49	MSE	MET	MODIFIED RESIDUE	UNP P06704
C	76	MSE	MET	MODIFIED RESIDUE	UNP P06704
C	85	MSE	MET	MODIFIED RESIDUE	UNP P06704
C	137	MSE	MET	MODIFIED RESIDUE	UNP P06704

- Molecule 2 is a protein called SFI1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	83	Total	C	N	O	Se	0	0	0
			704	450	124	128	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	213	GLY	-	CLONING ARTIFACT	UNP Q12369
D	214	PRO	-	CLONING ARTIFACT	UNP Q12369
D	215	LEU	-	CLONING ARTIFACT	UNP Q12369
D	216	GLY	-	CLONING ARTIFACT	UNP Q12369
D	217	SER	-	CLONING ARTIFACT	UNP Q12369
D	250	MSE	MET	MODIFIED RESIDUE	UNP Q12369
D	278	PHE	LEU	SEE REMARK 999	UNP Q12369
D	293	MSE	MET	MODIFIED RESIDUE	UNP Q12369

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

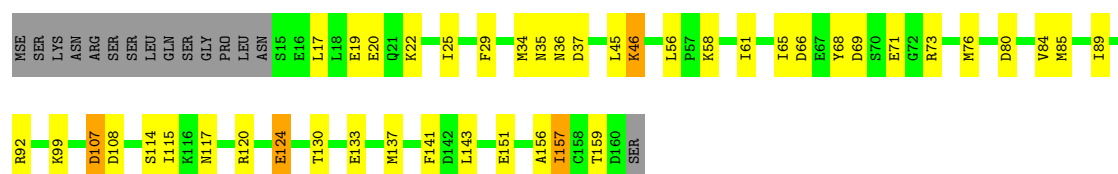
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	D	2	Total	O	0	0
			2	2		

### 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 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.

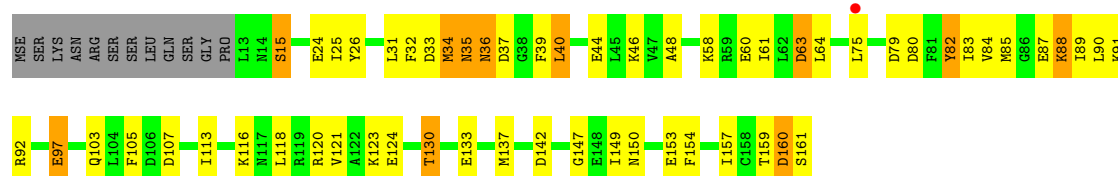
#### • Molecule 1: Cell division control protein 31

Chain A:



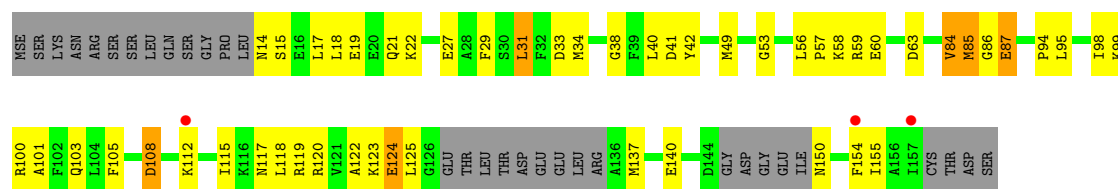
#### • Molecule 1: Cell division control protein 31

Chain B:



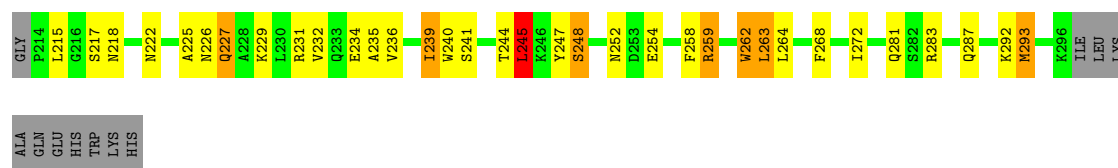
#### • Molecule 1: Cell division control protein 31

Chain C:



#### • Molecule 2: SFI1p

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.28Å 92.96Å 189.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.49 – 3.00 52.81 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (94.49-3.00) 99.5 (52.81-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.259 , 0.299 0.316 , 0.354	Depositor DCC
$R_{free}$ test set	782 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	110.9	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 15727 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.44	0/1218	0.57	0/1624
1	B	0.51	0/1240	0.71	1/1654 (0.1%)
1	C	0.44	0/1094	0.56	0/1453
2	D	0.59	0/718	0.69	1/961 (0.1%)
All	All	0.49	0/4270	0.63	2/5692 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	LEU	CA-CB-CG	6.04	129.19	115.30
2	D	245	LEU	CA-CB-CG	-5.15	103.46	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1205	0	1160	31	1
1	B	1227	0	1181	38	0
1	C	1083	0	1050	35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	704	0	685	32	1
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
All	All	4230	0	4076	118	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:34:MSE:CE	2:D:281:GLN:HG3	2.05	0.86
1:C:49:MSE:HE1	1:C:56:LEU:HD11	1.59	0.84
1:C:60:GLU:O	1:C:63:ASP:HB2	1.83	0.79
1:B:24:GLU:HG3	2:D:262:TRP:HD1	1.47	0.79
1:A:137:MSE:HA	2:D:245:LEU:HD13	1.68	0.76
1:A:137:MSE:HA	2:D:245:LEU:CD1	2.19	0.73
1:B:118:LEU:HD11	1:B:137:MSE:HE1	1.68	0.73
1:C:34:MSE:HE3	2:D:281:GLN:HG3	1.69	0.73
1:A:130:THR:HG23	1:A:133:GLU:H	1.58	0.69
1:B:154:PHE:HA	1:B:157:ILE:HD12	1.75	0.68
2:D:248:SER:O	2:D:252:ASN:HB2	1.94	0.68
1:A:141:PHE:HZ	2:D:244:THR:HG21	1.60	0.66
1:C:49:MSE:HE1	1:C:56:LEU:CD1	2.26	0.64
1:B:118:LEU:HD21	1:B:137:MSE:HE2	1.79	0.64
1:B:39:PHE:HB3	1:B:75:LEU:HD13	1.78	0.64
1:C:49:MSE:SE	1:C:85:MSE:HE1	2.48	0.64
1:C:99:LYS:O	1:C:103:GLN:HG2	1.97	0.64
1:B:35:ASN:HD21	1:B:37:ASP:CG	2.00	0.64
1:B:89:ILE:O	1:B:92:ARG:HB3	1.99	0.63
1:C:49:MSE:HE3	1:C:85:MSE:SE	2.49	0.62
1:B:89:ILE:O	1:B:92:ARG:CB	2.48	0.61
1:A:141:PHE:CZ	2:D:244:THR:HG21	2.38	0.58
1:A:141:PHE:HZ	2:D:244:THR:CG2	2.16	0.58
1:A:141:PHE:O	1:A:143:LEU:HG	2.04	0.58
1:B:25:ILE:HG21	1:B:82:TYR:HA	1.85	0.57
1:B:24:GLU:HG3	2:D:262:TRP:CD1	2.35	0.57
2:D:235:ALA:O	2:D:239:ILE:HG23	2.04	0.57
1:A:80:ASP:O	1:A:84:VAL:HG23	2.04	0.57
1:B:40:LEU:HD22	1:B:44:GLU:HB3	1.85	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:17:LEU:HB2	1:A:22:LYS:HE3	1.85	0.57
1:C:137:MSE:HB2	1:C:140:GLU:HB2	1.86	0.56
1:A:34:MSE:SE	2:D:218:ASN:HD21	2.39	0.56
1:C:84:VAL:O	1:C:87:GLU:HG3	2.06	0.56
1:B:149:ILE:HA	1:B:153:GLU:OE1	2.05	0.55
2:D:225:ALA:O	2:D:229:LYS:HG2	2.06	0.55
1:C:120:ARG:O	1:C:124:GLU:HB2	2.07	0.55
1:B:150:ASN:OD1	1:B:153:GLU:HG3	2.08	0.53
1:B:58:LYS:HA	1:B:61:ILE:HD12	1.89	0.53
1:B:118:LEU:HD11	1:B:137:MSE:CE	2.37	0.53
2:D:226:ASN:OD1	2:D:227:GLN:N	2.42	0.53
1:C:94:PRO:O	1:C:98:ILE:HG12	2.08	0.53
1:B:105:PHE:CD2	1:B:121:VAL:HG21	2.45	0.52
1:B:35:ASN:ND2	1:B:37:ASP:CG	2.63	0.52
1:C:105:PHE:O	1:C:117:ASN:HB3	2.10	0.51
1:C:124:GLU:HG2	2:D:287:GLN:HE22	1.76	0.51
1:A:29:PHE:O	1:A:29:PHE:CD2	2.64	0.51
2:D:268:PHE:O	2:D:272:ILE:HG22	2.10	0.51
1:B:142:ASP:OD2	1:B:147:GLY:N	2.37	0.51
1:C:123:LYS:C	1:C:125:LEU:H	2.14	0.51
2:D:258:PHE:O	2:D:259:ARG:C	2.49	0.51
1:A:84:VAL:HG12	1:A:85:MSE:HE2	1.92	0.50
1:B:87:GLU:HA	1:B:90:LEU:HD12	1.94	0.50
1:B:34:MSE:HE2	1:B:44:GLU:HG2	1.93	0.50
1:A:34:MSE:HE1	2:D:218:ASN:ND2	2.26	0.50
1:A:35:ASN:N	1:A:35:ASN:OD1	2.41	0.50
1:B:24:GLU:HA	2:D:262:TRP:HE1	1.79	0.48
1:B:35:ASN:O	1:B:36:ASN:HB2	2.14	0.48
1:A:137:MSE:SE	2:D:241:SER:HB2	2.63	0.48
1:A:89:ILE:O	1:A:92:ARG:HB2	2.14	0.48
1:A:99:LYS:HG2	1:A:151:GLU:OE1	2.12	0.48
2:D:292:LYS:HG3	2:D:293:MSE:H	1.78	0.48
1:C:94:PRO:HG2	1:C:95:LEU:HD12	1.96	0.48
1:C:119:ARG:HA	1:C:122:ALA:HB3	1.95	0.48
1:A:71:GLU:C	1:A:73:ARG:H	2.17	0.48
1:B:32:PHE:CD1	1:B:48:ALA:HA	2.49	0.48
1:B:120:ARG:HD2	1:B:124:GLU:OE1	2.15	0.47
1:A:108:ASP:OD2	1:A:108:ASP:N	2.47	0.47
1:A:35:ASN:O	1:A:37:ASP:N	2.47	0.47
2:D:292:LYS:HG3	2:D:293:MSE:N	2.30	0.47
1:C:18:LEU:HB3	1:C:21:GLN:OE1	2.14	0.47
1:A:107:ASP:OD1	1:A:120:ARG:NH2	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:115:ILE:HA	1:C:118:LEU:HB3	1.97	0.46
1:C:119:ARG:HG2	1:C:123:LYS:HD3	1.96	0.46
2:D:226:ASN:C	2:D:226:ASN:OD1	2.54	0.46
1:A:156:ALA:O	1:A:157:ILE:C	2.54	0.45
1:C:112:LYS:HE2	1:C:150:ASN:HD22	1.81	0.45
2:D:234:GLU:HG3	2:D:235:ALA:N	2.31	0.45
1:A:114:SER:O	1:A:117:ASN:HB2	2.16	0.45
1:A:89:ILE:O	1:A:92:ARG:CB	2.65	0.45
1:B:105:PHE:HB3	1:B:113:ILE:HG12	1.99	0.44
1:A:137:MSE:HG3	2:D:245:LEU:HD22	1.98	0.44
1:A:141:PHE:CZ	2:D:244:THR:CG2	2.98	0.44
2:D:262:TRP:HA	2:D:262:TRP:CE3	2.52	0.44
1:C:108:ASP:CG	1:C:117:ASN:HD21	2.20	0.44
1:A:45:LEU:HD23	1:A:61:ILE:HG23	2.00	0.44
1:C:58:LYS:O	1:C:59:ARG:C	2.55	0.44
1:C:29:PHE:CE1	1:C:40:LEU:HG	2.53	0.44
1:C:49:MSE:HE3	1:C:85:MSE:HE1	2.00	0.44
1:C:84:VAL:O	1:C:86:GLY:N	2.51	0.44
1:C:84:VAL:HG12	1:C:85:MSE:N	2.33	0.44
1:A:46:LYS:HG2	1:A:61:ILE:CD1	2.47	0.43
1:C:33:ASP:OD2	1:C:38:GLY:N	2.51	0.43
1:C:19:GLU:HA	1:C:22:LYS:HD2	1.99	0.43
1:C:101:ALA:HB2	2:D:293:MSE:HE3	2.00	0.43
2:D:234:GLU:HG3	2:D:235:ALA:H	1.83	0.43
1:B:123:LYS:HB2	1:B:123:LYS:HE3	1.83	0.43
1:B:60:GLU:HA	1:B:63:ASP:HB2	2.00	0.43
1:B:160:ASP:O	1:B:161:SER:CB	2.67	0.43
2:D:217:SER:HB3	2:D:218:ASN:H	1.72	0.42
1:C:155:ILE:H	1:C:155:ILE:HG13	1.58	0.42
1:A:65:ILE:O	1:A:69:ASP:HB2	2.20	0.42
1:B:46:LYS:HG3	1:B:61:ILE:HD13	2.01	0.42
1:B:85:MSE:HA	1:B:88:LYS:HB2	2.02	0.42
1:C:53:GLY:O	1:C:100:ARG:HD2	2.20	0.42
1:B:87:GLU:O	1:B:91:LYS:HG2	2.19	0.42
1:C:49:MSE:CE	1:C:85:MSE:HE1	2.50	0.41
1:B:32:PHE:HD1	1:B:48:ALA:HA	1.85	0.41
1:C:41:ASP:O	1:C:42:TYR:C	2.59	0.41
1:B:80:ASP:O	1:B:84:VAL:HG23	2.21	0.41
1:B:97:GLU:HG3	2:D:263:LEU:HD11	2.01	0.41
1:A:120:ARG:O	1:A:124:GLU:HB2	2.21	0.41
1:B:130:THR:HG22	1:B:133:GLU:HG3	2.02	0.41
2:D:240:TRP:CD1	2:D:240:TRP:C	2.94	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:27:GLU:O	1:C:31:LEU:HB2	2.20	0.41
1:A:68:TYR:HB2	1:A:76:MSE:HE3	2.02	0.40
1:B:120:ARG:HB3	1:B:120:ARG:HE	1.67	0.40
1:B:89:ILE:O	1:B:92:ARG:HB2	2.21	0.40
1:B:83:ILE:O	1:B:84:VAL:C	2.60	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	Distance(Å)	Clash(Å)
1:A:19:GLU:OE1	2:D:247:TYR:OH[3.656]	2.14	0.06

## 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	144/161 (89%)	133 (92%)	8 (6%)	3 (2%)	11	47
1	B	147/161 (91%)	125 (85%)	16 (11%)	6 (4%)	4	24
1	C	124/161 (77%)	105 (85%)	15 (12%)	4 (3%)	6	33
2	D	81/94 (86%)	63 (78%)	17 (21%)	1 (1%)	19	64
All	All	496/577 (86%)	426 (86%)	56 (11%)	14 (3%)	8	37

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	B	15	SER
1	B	33	ASP
1	C	84	VAL
1	B	36	ASN
1	B	82	TYR
1	C	85	MSE
1	B	26	TYR
1	B	160	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	124	GLU
2	D	259	ARG
1	C	57	PRO
1	A	157	ILE
1	A	25	ILE

### 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	131/139 (94%)	122 (93%)	9 (7%)	22	62
1	B	134/139 (96%)	120 (90%)	14 (10%)	10	37
1	C	117/139 (84%)	110 (94%)	7 (6%)	27	69
2	D	74/81 (91%)	59 (80%)	15 (20%)	2	9
All	All	456/498 (92%)	411 (90%)	45 (10%)	11	40

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	46	LYS
1	A	56	LEU
1	A	58	LYS
1	A	66	ASP
1	A	107	ASP
1	A	115	ILE
1	A	124	GLU
1	A	159	THR
1	B	15	SER
1	B	31	LEU
1	B	34	MSE
1	B	35	ASN
1	B	63	ASP
1	B	64	LEU
1	B	79	ASP
1	B	88	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	97	GLU
1	B	103	GLN
1	B	107	ASP
1	B	116	LYS
1	B	130	THR
1	B	159	THR
1	C	14	ASN
1	C	15	SER
1	C	17	LEU
1	C	31	LEU
1	C	87	GLU
1	C	108	ASP
1	C	154	PHE
2	D	215	LEU
2	D	222	ASN
2	D	227	GLN
2	D	231	ARG
2	D	232	VAL
2	D	236	VAL
2	D	239	ILE
2	D	245	LEU
2	D	248	SER
2	D	254	GLU
2	D	262	TRP
2	D	263	LEU
2	D	264	LEU
2	D	283	ARG
2	D	293	MSE

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

Mol	Chain	Res	Type
1	B	35	ASN
2	D	218	ASN
2	D	276	GLN
2	D	287	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 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.

## 5.7 Other polymers ⓘ

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	146/161 (90%)	0.12	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	106, 114, 124, 126	0
1	B	149/161 (92%)	0.24	1 (0%) <span style="border: 1px solid blue; padding: 2px;">84</span> <span style="border: 1px solid red; padding: 2px;">28</span>	101, 113, 123, 142	0
1	C	130/161 (80%)	0.35	3 (2%) <span style="border: 1px solid blue; padding: 2px;">57</span> <span style="border: 1px solid red; padding: 2px;">12</span>	102, 111, 122, 134	0
2	D	83/94 (88%)	0.26	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	98, 115, 143, 146	0
All	All	508/577 (88%)	0.24	4 (0%) <span style="border: 1px solid blue; padding: 2px;">83</span> <span style="border: 1px solid red; padding: 2px;">26</span>	98, 113, 130, 146	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	ILE	2.8
1	C	112	LYS	2.7
1	C	154	PHE	2.2
1	B	75	LEU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	C	162	1/1	0.20	-0.36	85,85,85,85	0
3	CA	B	162	1/1	0.16	-0.38	136,136,136,136	0
3	CA	A	162	1/1	0.16	-0.61	110,110,110,110	0
3	CA	B	164	1/1	0.21	-0.93	78,78,78,78	0
3	CA	A	164	1/1	0.06	-1.25	116,116,116,116	0
3	CA	A	163	1/1	0.06	-1.39	140,140,140,140	0
3	CA	B	163	1/1	0.12	-2.03	125,125,125,125	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.