



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2021 – 05:20 AM BST

PDB ID : 5BYH  
Title : Crystal Structure of Escherichia coli RNA polymerase - Sigma54 Holoenzyme complex  
Authors : Zhang, X.; Buck, M.; Darbari, V.C.; Yang, Y.; Zhang, N.; Lu, D.; Glyde, R.; Wang, Y.; Winkelman, J.; Gourse, R.L.; Murakami, K.S.  
Deposited on : 2015-06-10  
Resolution : 3.76 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 : 2.20  
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) : 2.20

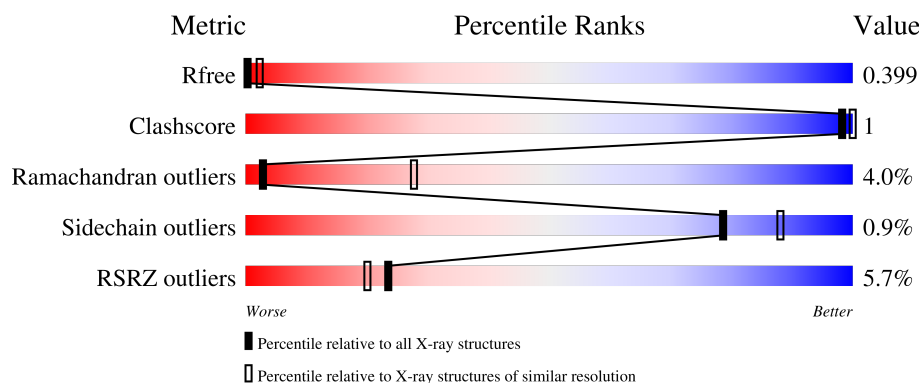
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.76 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	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>2%</div> <div>87%</div> <div>5%</div> <div>7%</div> </div>
1	B	329	<div> <div>5%</div> <div>64%</div> <div>34%</div> </div>
2	C	1342	<div> <div>7%</div> <div>95%</div> <div>2%</div> </div>
3	D	1407	<div> <div>4%</div> <div>93%</div> <div>3%</div> </div>
4	E	91	<div> <div>5%</div> <div>87%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
5	M	477	<div><div></div><div>8%</div><div></div><div>77%</div><div></div><div>9%</div><div>..</div><div>12%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22900 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			1975	1233	346	391	5			
1	B	216	Total	C	N	O	S	0	0	0
			1485	917	271	292	5			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1319	Total	C	N	O	S	0	1	0
			8347	5174	1507	1642	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1372	Total	C	N	O	S	0	0	0
			7824	4771	1488	1552	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	79	Total	C	N	O	S	0	0	0
			623	379	116	127	1			

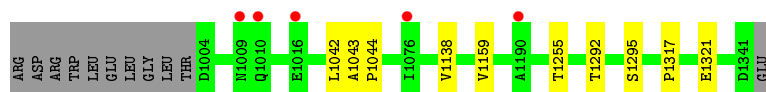
- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	M	421	Total	C	N	O	S	Se	0	0	0
			2645	1649	457	530	1	8			

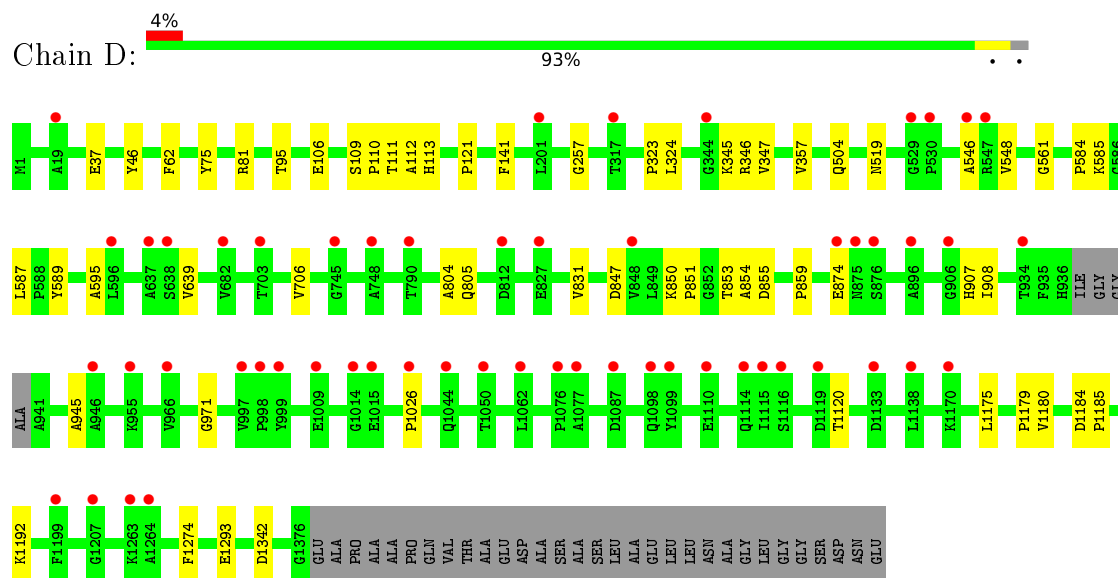
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total 1	Zn 1	0	0

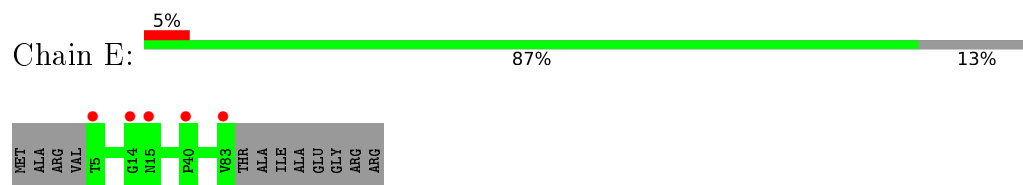




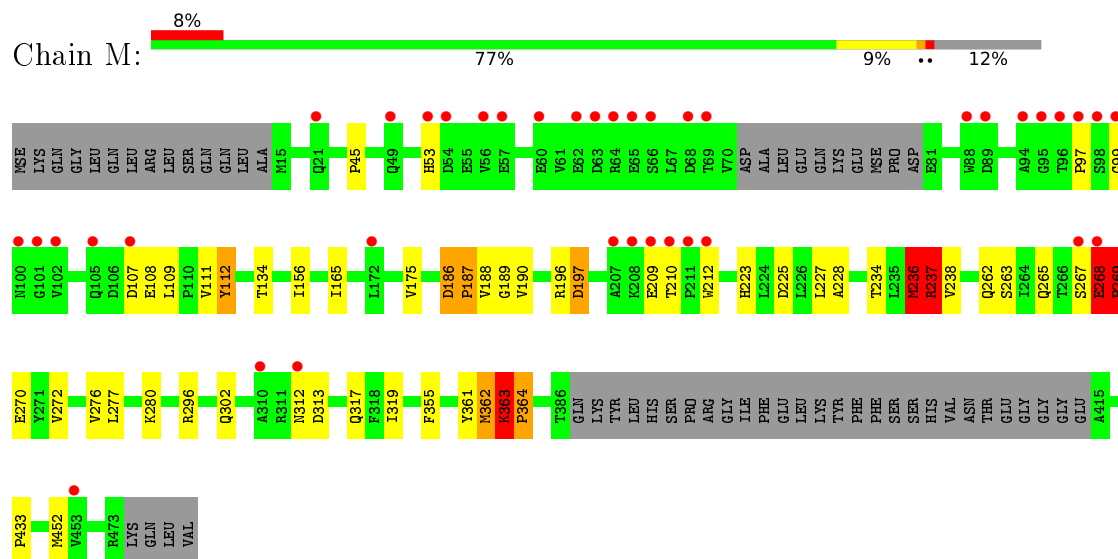
- Molecule 3: DNA-directed RNA polymerase subunit beta'



- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma-54 factor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.48 Å   151.52 Å   195.28 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.64 – 3.76 29.64 – 3.76	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.64-3.76) 98.5 (29.64-3.76)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 3.75 Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.2	Depositor
R, $R_{free}$	0.346 , 0.353 0.388 , 0.399	Depositor DCC
$R_{free}$ test set	3077 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	142.0	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 186.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	22900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: ZN

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	0.37	0/1999	0.58	0/2754
1	B	0.37	0/1502	0.57	0/2052
2	C	0.35	0/8473	0.54	2/11640 (0.0%)
3	D	0.34	0/7889	0.52	0/10883
4	E	0.36	0/625	0.52	0/842
5	M	0.42	0/2668	0.73	3/3672 (0.1%)
All	All	0.36	0/23156	0.56	5/31843 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
5	M	0	5
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	M	362	MSE	C-N-CA	6.49	137.92	121.70
5	M	236	MSE	C-N-CA	6.28	137.41	121.70
2	C	841	ARG	C-N-CA	5.63	135.78	121.70
2	C	58	PRO	N-CA-C	-5.49	97.84	112.10
5	M	362	MSE	N-CA-C	5.21	125.06	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	PHE	Mainchain
5	M	268	GLU	Peptide,Mainchain
5	M	269	PRO	Mainchain
5	M	362	MSE	Peptide
5	M	363	LYS	Mainchain

## 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	1975	0	1687	2	0
1	B	1485	0	1322	1	0
2	C	8347	0	6487	3	0
3	D	7824	0	5283	2	0
4	E	623	0	622	0	0
5	M	2645	0	2081	17	0
6	D	1	0	0	0	0
All	All	22900	0	17482	24	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 1.

All (24) 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)
5:M:363:LYS:HB3	5:M:364:PRO:CD	2.09	0.81
5:M:268:GLU:HG3	5:M:269:PRO:HD3	1.70	0.71
5:M:268:GLU:CG	5:M:269:PRO:HD3	2.20	0.70
5:M:363:LYS:HB3	5:M:364:PRO:HD3	1.88	0.55
5:M:268:GLU:CG	5:M:269:PRO:CD	2.89	0.51
5:M:223:HIS:O	5:M:228:ALA:HB3	2.12	0.49
2:C:733:VAL:HG12	2:C:750:ILE:HG22	1.96	0.48
5:M:363:LYS:O	5:M:364:PRO:C	2.51	0.48
5:M:268:GLU:HG3	5:M:269:PRO:CD	2.44	0.46
5:M:268:GLU:CB	5:M:269:PRO:CD	2.93	0.46
5:M:268:GLU:HB3	5:M:269:PRO:HD2	1.97	0.46
5:M:363:LYS:CB	5:M:364:PRO:CD	2.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:269:PRO:HB2	5:M:270:GLU:H	1.45	0.44
5:M:186:ASP:HB3	5:M:187:PRO:HD3	2.00	0.44
5:M:268:GLU:HB3	5:M:269:PRO:CD	2.48	0.44
2:C:257:ALA:HB2	2:C:285:ILE:HG22	1.99	0.43
5:M:236:MSE:HB3	5:M:237:ARG:H	1.55	0.42
1:A:126:PRO:HD2	1:A:127:GLN:OE1	2.20	0.42
3:D:46:TYR:HB3	5:M:268:GLU:HG2	2.02	0.42
1:A:125:LYS:HD2	1:A:128:HIS:HB2	2.01	0.41
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	2.02	0.41
5:M:267:SER:O	5:M:268:GLU:O	2.40	0.41
1:B:179:PRO:HA	1:B:209:GLY:HA3	2.03	0.40
3:D:1026:PRO:HB3	3:D:1120:THR:HG23	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	301/329 (92%)	247 (82%)	43 (14%)	11 (4%)	3	29
1	B	212/329 (64%)	186 (88%)	23 (11%)	3 (1%)	11	46
2	C	1312/1342 (98%)	1106 (84%)	173 (13%)	33 (2%)	5	36
3	D	1368/1407 (97%)	1155 (84%)	159 (12%)	54 (4%)	3	28
4	E	77/91 (85%)	72 (94%)	5 (6%)	0	100	100
5	M	415/477 (87%)	298 (72%)	70 (17%)	47 (11%)	0	6
All	All	3685/3975 (93%)	3064 (83%)	473 (13%)	148 (4%)	3	28

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	57	PHE

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Mol	Chain	Res	Type
2	C	121	GLU
2	C	555	TYR
2	C	842	ASP
2	C	887	VAL
3	D	81	ARG
3	D	110	PRO
3	D	323	PRO
3	D	831	VAL
3	D	859	PRO
3	D	1179	PRO
5	M	109	LEU
5	M	134	THR
5	M	165	ILE
5	M	175	VAL
5	M	187	PRO
5	M	197	ASP
5	M	227	LEU
5	M	237	ARG
5	M	269	PRO
5	M	277	LEU
5	M	363	LYS
5	M	364	PRO
1	A	112	ALA
1	A	113	ALA
2	C	58	PRO
2	C	338	THR
2	C	488	MET
2	C	490	GLN
3	D	37	GLU
3	D	75	TYR
3	D	357	VAL
3	D	587	LEU
3	D	805	GLN
3	D	850	LYS
3	D	971	GLY
5	M	53	HIS
5	M	156	ILE
5	M	186	ASP
5	M	188	VAL
5	M	190	VAL
5	M	212	TRP
5	M	234	THR

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Mol	Chain	Res	Type
5	M	236	MSE
5	M	238	VAL
5	M	276	VAL
5	M	312	ASN
5	M	317	GLN
5	M	452	MSE
1	A	111	THR
1	A	193	GLU
1	A	317	ARG
2	C	748	ILE
2	C	818	VAL
2	C	1042	LEU
2	C	1292	THR
3	D	111	THR
3	D	347	VAL
3	D	548	VAL
3	D	585	LYS
3	D	639	VAL
3	D	847	ASP
3	D	854	ALA
3	D	855	ASP
3	D	908	ILE
3	D	1185	PRO
3	D	1274	PHE
5	M	107	ASP
5	M	112	TYR
5	M	189	GLY
5	M	196	ARG
5	M	209	GLU
5	M	265	GLN
5	M	296	ARG
5	M	313	ASP
1	A	114	ASP
1	A	163	GLU
1	A	252	ILE
1	B	138	ALA
1	B	193	GLU
2	C	98	VAL
2	C	851	THR
2	C	853	ASP
2	C	854	ILE
2	C	886	LYS

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Mol	Chain	Res	Type
2	C	1138	VAL
2	C	1295	SER
3	D	112	ALA
3	D	113	HIS
3	D	257	GLY
3	D	346	ARG
3	D	519	ASN
3	D	595	ALA
3	D	804	ALA
3	D	851	PRO
3	D	853	THR
3	D	1192	LYS
3	D	1293	GLU
3	D	1342	ASP
5	M	97	PRO
5	M	99	GLY
5	M	210	THR
5	M	263	SER
5	M	302	GLN
5	M	433	PRO
1	A	14	VAL
1	A	320	ASN
2	C	117	ILE
2	C	311	CYS
2	C	1159	VAL
2	C	1255	THR
2	C	1321	GLU
3	D	62	PHE
3	D	95	THR
3	D	106	GLU
3	D	141	PHE
3	D	324	LEU
3	D	345	LYS
3	D	504	GLN
3	D	589	TYR
3	D	874	GLU
3	D	945	ALA
3	D	1175	LEU
5	M	108	GLU
5	M	262	GLN
5	M	268	GLU
5	M	280	LYS

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Mol	Chain	Res	Type
1	B	13	LEU
2	C	111	GLU
2	C	329	GLY
2	C	596	ASP
2	C	655	VAL
2	C	746	ALA
2	C	894	GLN
3	D	546	ALA
3	D	706	VAL
3	D	1180	VAL
5	M	45	PRO
2	C	228	VAL
5	M	111	VAL
3	D	584	PRO
3	D	1184	ASP
5	M	319	ILE
1	A	326	ILE
2	C	1317	PRO
3	D	121	PRO
3	D	561	GLY
5	M	272	VAL

### 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	159/286 (56%)	156 (98%)	3 (2%)	57	76
1	B	130/286 (46%)	129 (99%)	1 (1%)	81	89
2	C	567/1157 (49%)	567 (100%)	0	100	100
3	D	332/1168 (28%)	330 (99%)	2 (1%)	86	93
4	E	66/75 (88%)	66 (100%)	0	100	100
5	M	186/412 (45%)	179 (96%)	7 (4%)	33	61
All	All	1440/3384 (43%)	1427 (99%)	13 (1%)	78	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	178	SER
1	A	314	LEU
1	B	133	LEU
3	D	109	SER
3	D	907	HIS
5	M	112	TYR
5	M	197	ASP
5	M	225	ASP
5	M	237	ARG
5	M	268	GLU
5	M	355	PHE
5	M	361	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
2	C	1244	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	967:LEU	C	968:GLU	N	4.69
1	C	941:LYS	C	942:ASP	N	3.24

## 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	305/329 (92%)	0.07	7 (2%) 60 55	110, 223, 287, 299	0
1	B	216/329 (65%)	0.21	15 (6%) 16 13	31, 239, 294, 300	0
2	C	1319/1342 (98%)	0.16	89 (6%) 17 14	71, 208, 294, 297	0
3	D	1372/1407 (97%)	-0.10	55 (4%) 38 33	32, 195, 300, 300	0
4	E	79/91 (86%)	0.15	5 (6%) 20 16	130, 170, 281, 289	0
5	M	412/477 (86%)	0.25	39 (9%) 8 7	111, 214, 298, 300	0
All	All	3703/3975 (93%)	0.07	210 (5%) 23 20	31, 208, 300, 300	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	251	ALA	12.1
2	C	298	ALA	11.1
3	D	848	VAL	10.2
5	M	101	GLY	8.4
2	C	238	GLN	7.9
2	C	299	LYS	7.4
5	M	96	THR	7.0
2	C	252	SER	6.7
2	C	332	ARG	6.6
2	C	334	GLU	6.4
2	C	266	GLY	6.3
2	C	333	ILE	6.1
5	M	94	ALA	5.9
2	C	259	GLY	5.9
5	M	100	ASN	5.8
2	C	260	LYS	5.7
5	M	95	GLY	5.6
2	C	318	SER	5.4
5	M	97	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
3	D	1207	GLY	5.3
2	C	257	ALA	5.2
2	C	234	ASP	5.1
2	C	248	GLY	4.9
2	C	253	PHE	4.8
2	C	910	ALA	4.7
2	C	309	LEU	4.6
2	C	258	ASN	4.4
2	C	267	ARG	4.3
5	M	68	ASP	4.3
1	B	97	GLU	4.2
2	C	344	GLY	4.2
2	C	311	CYS	4.1
3	D	966	VAL	4.1
2	C	421	SER	4.1
5	M	56	VAL	4.0
5	M	208	LYS	4.0
2	C	301	TYR	4.0
2	C	235	ASN	3.9
5	M	102	VAL	3.9
1	B	194	GLN	3.9
2	C	275	ARG	3.8
2	C	254	ASP	3.8
5	M	211	PRO	3.8
2	C	276	GLN	3.7
3	D	547	ARG	3.7
2	C	330	HIS	3.7
1	A	160	HIS	3.7
3	D	1115	ILE	3.7
3	D	1077	ALA	3.7
5	M	69	THR	3.6
2	C	250	THR	3.6
3	D	1014	GLY	3.6
3	D	1116	SER	3.6
2	C	239	MET	3.6
2	C	874	GLY	3.6
3	D	827	GLU	3.6
2	C	1016	GLU	3.6
2	C	911	SER	3.6
2	C	261	VAL	3.6
5	M	88	TRP	3.5
2	C	256	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	634	VAL	3.5
2	C	262	TYR	3.5
2	C	269	ILE	3.5
1	A	52	PRO	3.4
1	B	175	ALA	3.4
5	M	54	ASP	3.4
3	D	1099	TYR	3.4
5	M	312	ASN	3.3
2	C	338	THR	3.3
2	C	893	THR	3.3
5	M	268	GLU	3.3
5	M	63	ASP	3.3
3	D	1015	GLU	3.2
1	B	68	TYR	3.1
2	C	317	LEU	3.1
3	D	1087	ASP	3.1
4	E	40	PRO	3.1
2	C	726	TYR	3.0
5	M	53	HIS	3.0
2	C	630	VAL	3.0
5	M	210	THR	3.0
2	C	231	GLU	3.0
3	D	1098	GLN	3.0
2	C	390	PHE	3.0
5	M	209	GLU	2.9
2	C	727	VAL	2.9
2	C	170	VAL	2.9
1	B	96	ASP	2.9
3	D	998	PRO	2.9
1	B	192	VAL	2.9
3	D	638	SER	2.9
2	C	255	ILE	2.9
3	D	1076	PRO	2.9
5	M	310	ALA	2.9
3	D	703	THR	2.9
2	C	233	ARG	2.9
3	D	529	GLY	2.9
1	A	69	SER	2.9
3	D	896	ALA	2.9
3	D	19	ALA	2.9
1	B	58	GLU	2.8
5	M	21	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	317	THR	2.8
5	M	105	GLN	2.8
5	M	49	GLN	2.8
5	M	57	GLU	2.8
2	C	237	LEU	2.8
3	D	1110	GLU	2.8
2	C	376	PRO	2.8
2	C	300	ASP	2.8
5	M	207	ALA	2.7
1	B	54	CYS	2.7
2	C	691	PRO	2.7
3	D	1133	ASP	2.7
2	C	286	GLU	2.7
1	A	209	GLY	2.7
5	M	65	GLU	2.7
1	A	70	THR	2.7
3	D	530	PRO	2.7
1	B	57	THR	2.7
5	M	66	SER	2.7
3	D	748	ALA	2.7
3	D	934	THR	2.7
3	D	1026	PRO	2.7
5	M	98	SER	2.7
1	B	66	HIS	2.6
1	A	205	MET	2.6
3	D	999	TYR	2.6
5	M	62	GLU	2.6
2	C	1190	ALA	2.6
2	C	310	ILE	2.6
3	D	682	VAL	2.6
3	D	876	SER	2.6
3	D	596	LEU	2.6
1	B	59	VAL	2.6
3	D	1263	LYS	2.6
2	C	342	ASP	2.6
3	D	546	ALA	2.6
1	B	145	LYS	2.5
2	C	343	HIS	2.5
4	E	5	THR	2.5
2	C	225	PHE	2.5
2	C	230	PHE	2.5
3	D	1170	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	264	GLU	2.5
2	C	350	THR	2.5
2	C	605	TYR	2.5
2	C	335	THR	2.5
2	C	336	LEU	2.5
2	C	229	ILE	2.5
4	E	15	ASN	2.5
3	D	1009	GLU	2.4
5	M	267	SER	2.4
5	M	64	ARG	2.4
1	B	135	ASP	2.4
2	C	105	TYR	2.4
3	D	1050	THR	2.4
3	D	955	LYS	2.4
5	M	212	TRP	2.4
3	D	1114	GLN	2.4
1	A	53	GLY	2.4
3	D	997	VAL	2.4
2	C	297	VAL	2.4
2	C	942	ASP	2.4
2	C	420	LEU	2.3
5	M	99	GLY	2.3
2	C	272	ARG	2.3
2	C	1010	GLN	2.3
5	M	60	GLU	2.3
2	C	292	ILE	2.3
5	M	453	VAL	2.3
2	C	285	ILE	2.2
3	D	1062	LEU	2.2
3	D	1199	PHE	2.2
3	D	1119	ASP	2.2
3	D	946	ALA	2.2
2	C	236	LYS	2.2
2	C	337	PHE	2.2
2	C	391	SER	2.2
3	D	1044	GLN	2.2
5	M	89	ASP	2.2
2	C	1076	ILE	2.2
3	D	745	GLY	2.2
2	C	314	ASN	2.2
2	C	168	GLY	2.1
3	D	637	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
5	M	172	LEU	2.1
2	C	622	ASN	2.1
2	C	1009	ASN	2.1
4	E	14	GLY	2.1
1	B	98	VAL	2.1
3	D	1264	ALA	2.1
3	D	812	ASP	2.1
3	D	1138	LEU	2.1
3	D	201	LEU	2.1
2	C	304	GLU	2.1
3	D	344	GLY	2.1
3	D	906	GLY	2.1
5	M	107	ASP	2.1
3	D	875	ASN	2.1
2	C	265	LYS	2.0
2	C	803	ALA	2.0
3	D	790	THR	2.0
4	E	83	VAL	2.0
2	C	655	VAL	2.0
2	C	232	ILE	2.0
3	D	874	GLU	2.0
1	B	146	VAL	2.0
2	C	773	LEU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ZN	D	1501	1/1	0.86	0.32	268,268,268,268	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.