



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:21 PM GMT

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  
<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:

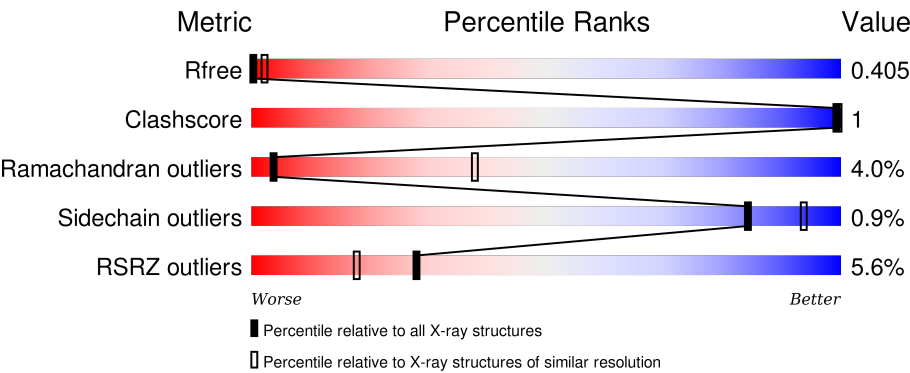
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

# 1 Overall quality at a glance i

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))
$R_{free}$	91344	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)

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	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>•</div><div>34%</div></div>
2	C	1342	<div><div>7%</div><div>95%</div><div>•</div><div>•</div></div>
3	D	1407	<div><div>4%</div><div>93%</div><div>•</div><div>•</div></div>
4	E	91	<div><div>4%</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	2	7			

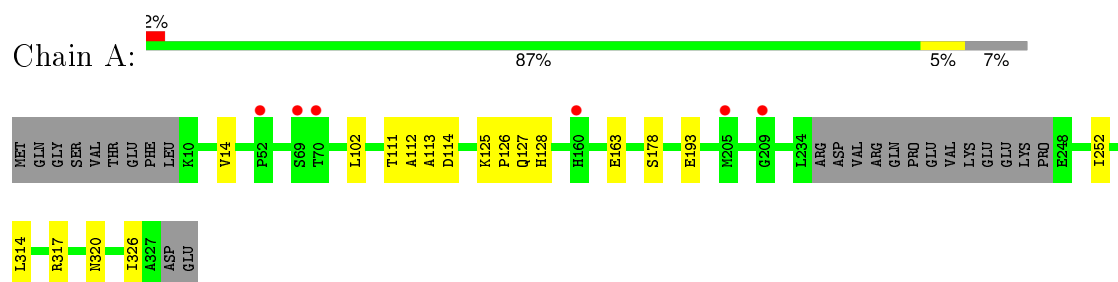
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

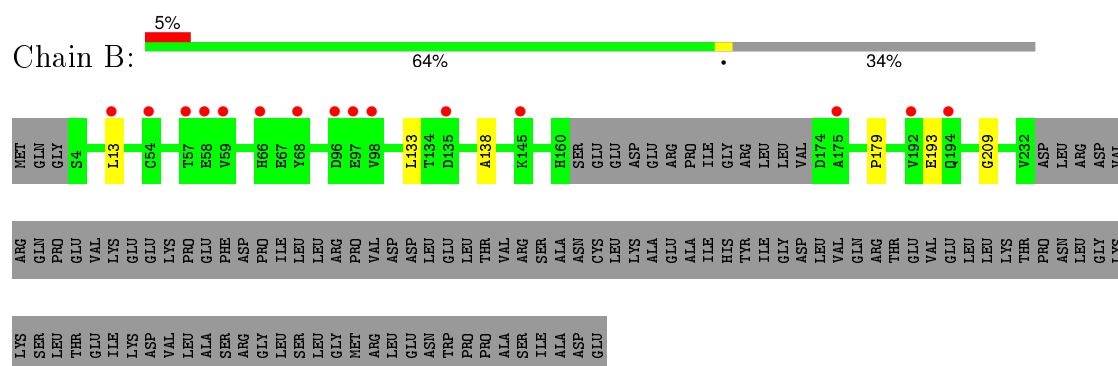
### 3 Residue-property plots [i](#)

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.

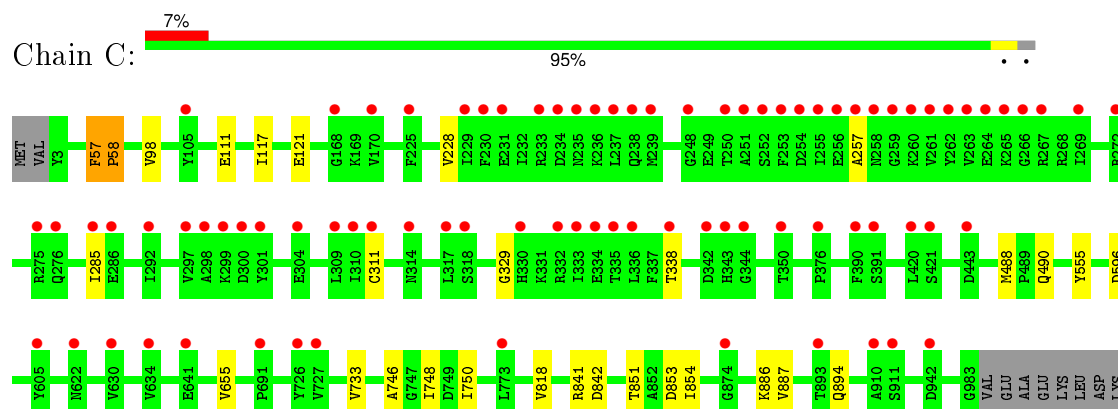
- Molecule 1: DNA-directed RNA polymerase subunit alpha

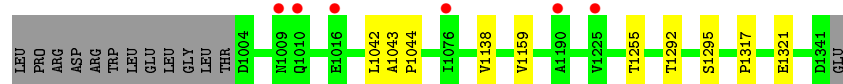


- Molecule 1: DNA-directed RNA polymerase subunit alpha

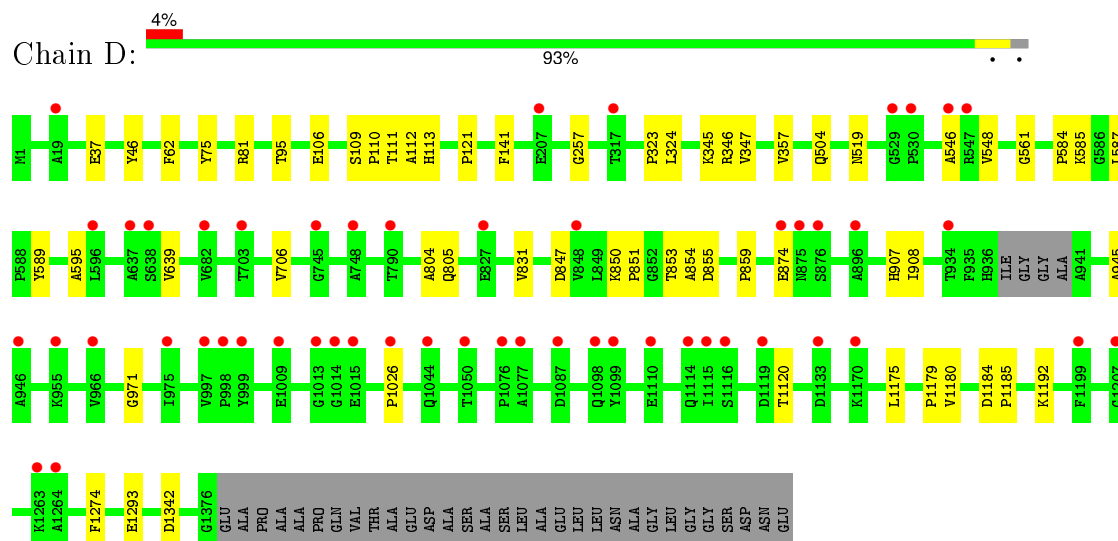


- Molecule 2: DNA-directed RNA polymerase subunit beta

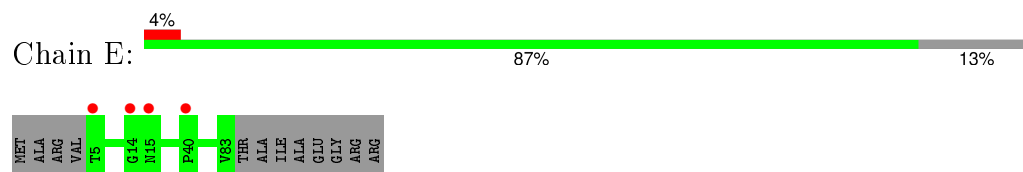




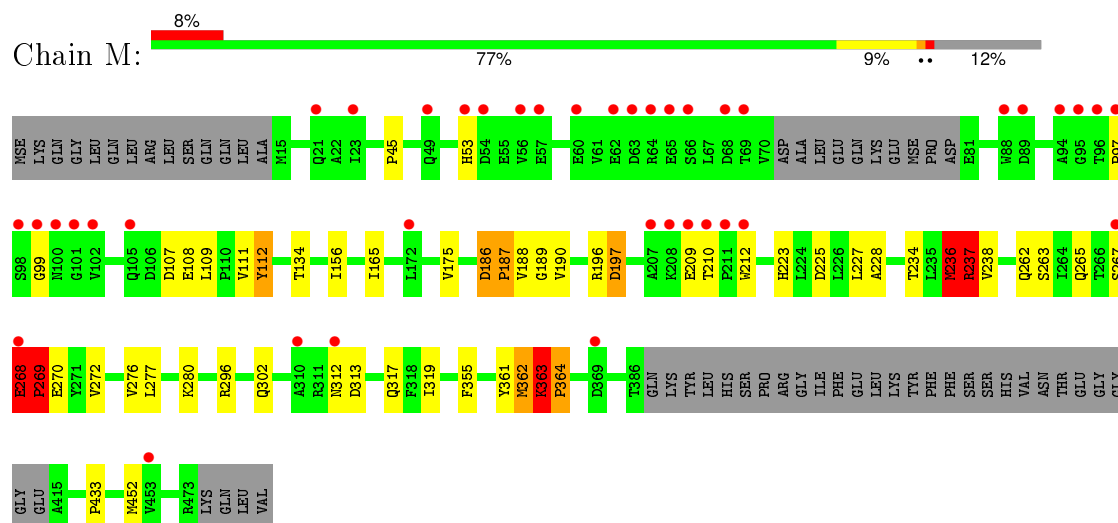
- Molecule 3: DNA-directed RNA polymerase subunit beta'



- 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, $\alpha$ , $\beta$ , $\gamma$	208.48Å 151.52Å 195.28Å 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 3.75Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.346 , 0.353 0.396 , 0.405	Depositor DCC
$R_{free}$ test set	3078 reflections (5.19%)	DCC
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 , 185.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 62410 reflections (0.002%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/2669	0.73	3/3675 (0.1%)
All	All	0.36	0/23157	0.56	5/31846 (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(°)	Ideal(°)
5	M	362	MSE	C-N-CA	6.49	137.92	121.70
5	M	236	MET	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	Mainchain,Peptide
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:268:GLU:HB3	5:M:269:PRO:CD	2.48	0.44
5:M:186:ASP:HB3	5:M:187:PRO:HD3	2.00	0.44
2:C:257:ALA:HB2	2:C:285:ILE:HG22	1.99	0.43
5:M:236:MET: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%)	4	40
1	B	212/329 (64%)	186 (88%)	23 (11%)	3 (1%)	14	59
2	C	1312/1342 (98%)	1106 (84%)	173 (13%)	33 (2%)	7	49
3	D	1368/1407 (97%)	1155 (84%)	159 (12%)	54 (4%)	4	38
4	E	77/91 (85%)	72 (94%)	5 (6%)	0	100	100
5	M	415/477 (87%)	298 (72%)	70 (17%)	47 (11%)	0	10
All	All	3685/3975 (93%)	3064 (83%)	473 (13%)	148 (4%)	4	38

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	MET
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%)	65	87
1	B	130/286 (46%)	129 (99%)	1 (1%)	86	95
2	C	567/1157 (49%)	567 (100%)	0	100	100
3	D	332/1168 (28%)	330 (99%)	2 (1%)	90	96
4	E	66/75 (88%)	66 (100%)	0	100	100
5	M	186/413 (45%)	179 (96%)	7 (4%)	40	76
All	All	1440/3385 (42%)	1427 (99%)	13 (1%)	84	94

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

Some 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 carbohydrates 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%)	0.06	6 (1%) 68 53	110, 223, 287, 299	0
1	B	216/329 (65%)	0.20	15 (6%) 20 12	31, 239, 294, 300	0
2	C	1319/1342 (98%)	0.16	89 (6%) 21 12	71, 208, 294, 297	0
3	D	1372/1407 (97%)	-0.10	52 (3%) 44 30	32, 195, 300, 300	0
4	E	79/91 (86%)	0.14	4 (5%) 32 21	130, 170, 281, 289	0
5	M	413/477 (86%)	0.25	40 (9%) 10 6	111, 214, 298, 300	0
All	All	3704/3975 (93%)	0.06	206 (5%) 28 18	31, 208, 300, 300	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	251	ALA	12.6
2	C	298	ALA	10.7
3	D	848	VAL	10.1
5	M	101	GLY	7.8
5	M	96	THR	7.2
2	C	238	GLN	7.0
2	C	299	LYS	6.9
2	C	266	GLY	6.8
2	C	252	SER	6.6
2	C	334	GLU	6.2
2	C	333	ILE	6.1
2	C	332	ARG	6.1
2	C	259	GLY	5.9
5	M	94	ALA	5.8
3	D	1207	GLY	5.6
5	M	100	ASN	5.6
5	M	95	GLY	5.5
2	C	248	GLY	5.3
2	C	257	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
2	C	318	SER	5.2
2	C	234	ASP	5.2
2	C	260	LYS	5.1
5	M	97	PRO	4.9
2	C	258	ASN	4.9
2	C	309	LEU	4.8
1	B	97	GLU	4.7
2	C	910	ALA	4.6
2	C	253	PHE	4.6
2	C	311	CYS	4.4
5	M	68	ASP	4.3
3	D	1077	ALA	4.3
2	C	267	ARG	4.2
3	D	966	VAL	4.2
2	C	344	GLY	4.1
5	M	208	LYS	3.9
3	D	547	ARG	3.9
2	C	254	ASP	3.9
5	M	54	ASP	3.9
3	D	1014	GLY	3.9
2	C	330	HIS	3.9
5	M	56	VAL	3.8
2	C	276	GLN	3.8
2	C	421	SER	3.8
2	C	235	ASN	3.8
2	C	301	TYR	3.8
5	M	102	VAL	3.8
5	M	211	PRO	3.8
2	C	275	ARG	3.7
1	B	194	GLN	3.6
2	C	1016	GLU	3.6
3	D	1115	ILE	3.6
5	M	69	THR	3.6
2	C	250	THR	3.6
5	M	268	GLU	3.5
1	A	52	PRO	3.5
5	M	312	ASN	3.4
1	A	160	HIS	3.4
3	D	1099	TYR	3.4
2	C	262	TYR	3.4
3	D	827	GLU	3.4
2	C	338	THR	3.4

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Mol	Chain	Res	Type	RSRZ
5	M	53	HIS	3.4
2	C	911	SER	3.3
2	C	634	VAL	3.3
2	C	874	GLY	3.3
3	D	1015	GLU	3.3
2	C	239	MET	3.3
2	C	390	PHE	3.3
2	C	261	VAL	3.2
1	B	175	ALA	3.2
2	C	237	LEU	3.2
2	C	269	ILE	3.2
3	D	1116	SER	3.1
5	M	49	GLN	3.1
4	E	40	PRO	3.1
5	M	21	GLN	3.1
5	M	88	TRP	3.1
5	M	63	ASP	3.1
2	C	317	LEU	3.0
2	C	170	VAL	3.0
2	C	255	ILE	3.0
2	C	893	THR	3.0
5	M	210	THR	3.0
2	C	310	ILE	3.0
2	C	225	PHE	3.0
2	C	727	VAL	2.9
3	D	896	ALA	2.9
1	B	96	ASP	2.9
5	M	209	GLU	2.9
1	B	58	GLU	2.9
3	D	1098	GLN	2.9
2	C	256	GLU	2.9
2	C	726	TYR	2.9
3	D	1114	GLN	2.9
1	B	68	TYR	2.9
1	A	70	THR	2.9
1	B	192	VAL	2.9
2	C	297	VAL	2.9
3	D	934	THR	2.8
2	C	691	PRO	2.8
1	A	69	SER	2.8
2	C	231	GLU	2.8
3	D	1076	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	1087	ASP	2.8
2	C	630	VAL	2.8
3	D	529	GLY	2.8
3	D	876	SER	2.8
5	M	98	SER	2.8
2	C	376	PRO	2.8
3	D	530	PRO	2.8
3	D	1110	GLU	2.8
3	D	638	SER	2.8
5	M	57	GLU	2.8
5	M	105	GLN	2.8
2	C	229	ILE	2.8
5	M	310	ALA	2.8
3	D	1263	LYS	2.7
3	D	19	ALA	2.7
3	D	596	LEU	2.7
3	D	1133	ASP	2.7
5	M	65	GLU	2.7
1	B	57	THR	2.7
1	A	205	MET	2.7
1	B	59	VAL	2.7
3	D	703	THR	2.6
5	M	207	ALA	2.6
3	D	998	PRO	2.6
2	C	605	TYR	2.6
2	C	264	GLU	2.6
2	C	300	ASP	2.6
1	B	98	VAL	2.6
1	A	209	GLY	2.6
2	C	233	ARG	2.6
3	D	955	LYS	2.6
1	B	54	CYS	2.6
2	C	272	ARG	2.6
3	D	1050	THR	2.5
3	D	1009	GLU	2.5
2	C	335	THR	2.5
2	C	391	SER	2.5
3	D	999	TYR	2.5
4	E	5	THR	2.5
2	C	1190	ALA	2.5
3	D	1026	PRO	2.5
5	M	99	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	546	ALA	2.5
1	B	66	HIS	2.5
3	D	748	ALA	2.5
5	M	267	SER	2.4
2	C	105	TYR	2.4
2	C	350	THR	2.4
3	D	317	THR	2.4
2	C	230	PHE	2.4
3	D	1170	LYS	2.4
5	M	62	GLU	2.4
5	M	66	SER	2.4
3	D	682	VAL	2.4
5	M	89	ASP	2.4
5	M	212	TRP	2.3
2	C	1010	GLN	2.3
3	D	1119	ASP	2.3
2	C	314	ASN	2.3
2	C	342	ASP	2.3
2	C	942	ASP	2.3
2	C	343	HIS	2.3
2	C	168	GLY	2.3
3	D	637	ALA	2.3
2	C	285	ILE	2.3
3	D	1013	GLY	2.3
5	M	64	ARG	2.3
2	C	420	LEU	2.2
2	C	292	ILE	2.2
1	B	135	ASP	2.2
2	C	1076	ILE	2.2
2	C	622	ASN	2.2
3	D	745	GLY	2.2
1	B	145	LYS	2.2
3	D	1264	ALA	2.2
4	E	15	ASN	2.2
3	D	946	ALA	2.2
2	C	1009	ASN	2.2
3	D	790	THR	2.2
3	D	874	GLU	2.1
3	D	1199	PHE	2.1
3	D	997	VAL	2.1
5	M	453	VAL	2.1
2	C	286	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
5	M	23	ILE	2.1
2	C	236	LYS	2.1
2	C	265	LYS	2.1
2	C	641	GLU	2.1
3	D	1044	GLN	2.1
2	C	263	VAL	2.1
2	C	1225	VAL	2.1
4	E	14	GLY	2.1
3	D	975	ILE	2.1
3	D	875	ASN	2.1
2	C	336	LEU	2.1
5	M	60	GLU	2.1
5	M	172	LEU	2.0
2	C	443	ASP	2.0
1	B	13	LEU	2.0
2	C	773	LEU	2.0
5	M	369	ASP	2.0
2	C	304	GLU	2.0
3	D	207	GLU	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( $\text{\AA}^2$ )	Q<0.9
6	ZN	D	1501	1/1	0.87	0.32	0.29	268,268,268,268	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.