



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:43 pm GMT

PDB ID : 3F1V  
Title : E. coli Beta Sliding Clamp, 148-153 Ala Mutant  
Authors : Cody, V.  
Deposited on : 2008-10-28  
Resolution : 1.77 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 : trunk28620  
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) : recalc28949

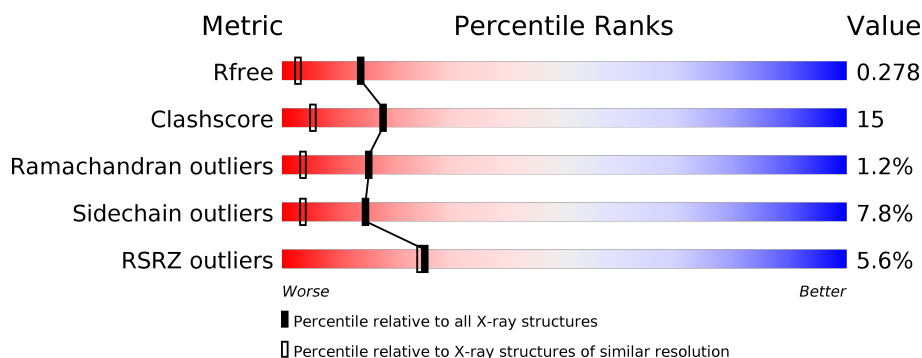
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	366	
1	B	366	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	368	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6029 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 polymerase III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	4	0
			2824	1775	492	538	19			
1	B	366	Total	C	N	O	S	0	3	0
			2824	1775	492	538	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ALA	HIS	ENGINEERED	UNP P0A988
A	149	ALA	GLN	ENGINEERED	UNP P0A988
A	150	ALA	ASP	ENGINEERED	UNP P0A988
A	151	ALA	VAL	ENGINEERED	UNP P0A988
A	152	ALA	ARG	ENGINEERED	UNP P0A988
B	148	ALA	HIS	ENGINEERED	UNP P0A988
B	149	ALA	GLN	ENGINEERED	UNP P0A988
B	150	ALA	ASP	ENGINEERED	UNP P0A988
B	151	ALA	VAL	ENGINEERED	UNP P0A988
B	152	ALA	ARG	ENGINEERED	UNP P0A988

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

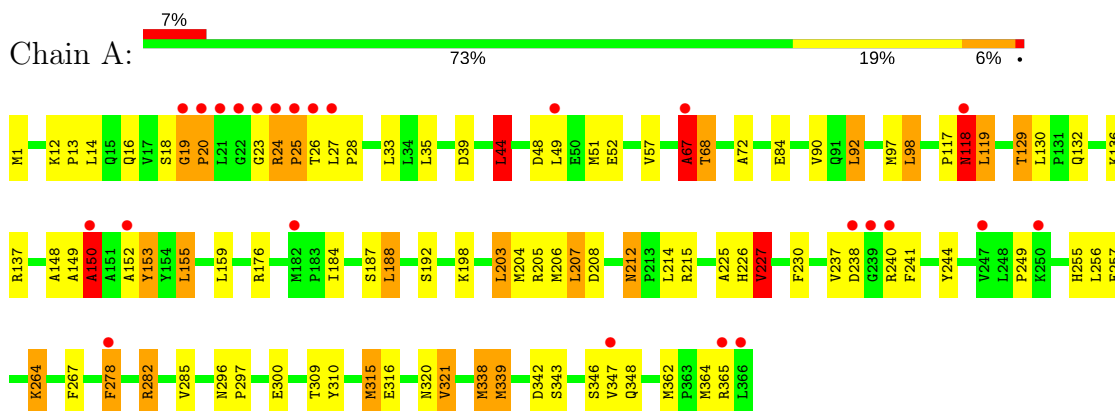
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total 173	O 173	0	0
4	B	205	Total 205	O 205	0	0

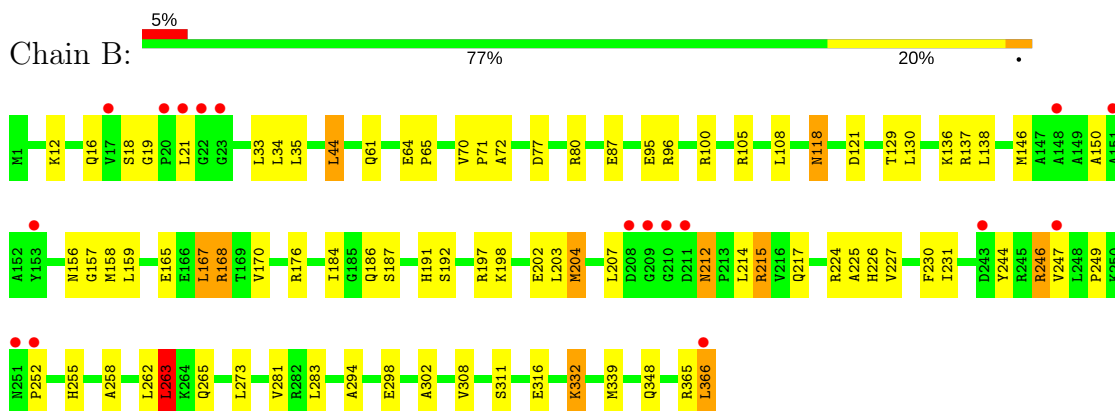
### 3 Residue-property plots

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: DNA polymerase III subunit beta



#### • Molecule 1: DNA polymerase III subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.84Å 64.47Å 72.11Å 73.83° 82.72° 83.76°	Depositor
Resolution (Å)	28.86 – 1.77 28.85 – 1.77	Depositor EDS
% Data completeness (in resolution range)	91.1 (28.86-1.77) 84.0 (28.85-1.77)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.282 0.214 , 0.278	Depositor DCC
$R_{free}$ test set	3131 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6029	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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: CA, 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	0.93	1/2872 (0.0%)	1.02	9/3888 (0.2%)
1	B	0.86	1/2872 (0.0%)	0.96	7/3888 (0.2%)
All	All	0.89	2/5744 (0.0%)	0.99	16/7776 (0.2%)

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
1	A	1	4
1	B	0	1
All	All	1	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	GLU	CB-CG	6.84	1.65	1.52
1	B	96	ARG	CB-CG	-5.07	1.38	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	LEU	CB-CG-CD1	-8.96	95.76	111.00
1	A	67	ALA	CB-CA-C	-7.82	98.37	110.10
1	A	118	ASN	N-CA-C	7.21	130.47	111.00
1	A	227	VAL	CB-CA-C	-6.69	98.69	111.40
1	A	19	GLY	N-CA-C	6.42	129.14	113.10
1	B	96	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	366	LEU	CA-CB-CG	6.34	129.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	PRO	C-N-CA	6.27	137.38	121.70
1	A	118	ASN	CB-CA-C	-6.26	97.88	110.40
1	A	44	LEU	CA-CB-CG	6.16	129.47	115.30
1	A	98	LEU	CA-CB-CG	5.87	128.81	115.30
1	B	263	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	34	LEU	CB-CG-CD1	5.65	120.61	111.00
1	A	67	ALA	N-CA-C	5.57	126.03	111.00
1	B	121	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	263	LEU	CB-CG-CD2	-5.24	102.09	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	149	ALA	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASN	Peptide
1	A	148	ALA	Peptide
1	A	150	ALA	Peptide
1	A	67	ALA	Peptide
1	B	365	ARG	Peptide

## 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	2824	0	2834	103	0
1	B	2824	0	2838	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	1	0	0	0	0
4	A	173	0	0	11	1
4	B	205	0	0	8	2
All	All	6029	0	5672	172	2

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 15.

All (172) 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:A:118:ASN:HB3	1:A:119:LEU:CA	1.65	1.23
1:A:184:ILE:HD11	1:A:188:LEU:HD11	1.26	1.10
1:A:267:PHE:HD1	1:A:321:VAL:CG1	1.66	1.09
1:A:90:VAL:HG11	1:A:97:MET:HE1	1.16	1.09
1:A:150:ALA:HA	1:A:152:ALA:H	1.16	1.08
1:A:118:ASN:HB3	1:A:119:LEU:HA	1.27	1.07
1:A:90:VAL:HG11	1:A:97:MET:CE	1.87	1.05
1:A:150:ALA:HA	1:A:152:ALA:N	1.73	1.03
1:A:118:ASN:CB	1:A:119:LEU:HA	1.90	1.02
1:A:12:LYS:HG2	1:A:13:PRO:HD3	1.41	1.01
1:A:267:PHE:HD1	1:A:321:VAL:HG12	1.24	1.00
1:A:90:VAL:CG1	1:A:97:MET:CE	2.38	1.00
1:B:215:ARG:HH11	1:B:215:ARG:HG2	1.25	0.99
1:A:90:VAL:CG1	1:A:97:MET:HE1	1.91	0.98
1:A:278:PHE:O	1:A:278:PHE:HD2	1.44	0.97
1:A:136:LYS:HD2	1:A:204:MET:HE1	1.42	0.96
1:A:267:PHE:CD1	1:A:321:VAL:CG1	2.50	0.94
1:A:118:ASN:CB	1:A:119:LEU:CA	2.46	0.93
1:A:255:HIS:HD2	1:A:339:MET:HE1	1.34	0.92
1:A:255:HIS:CD2	1:A:339:MET:CE	2.57	0.87
1:A:278:PHE:O	1:A:278:PHE:CD2	2.26	0.87
1:A:255:HIS:HD2	1:A:339:MET:CE	1.89	0.85
1:B:150:ALA:H	1:B:156:ASN:HD21	1.20	0.85
1:A:346:SER:OG	1:A:362:MET:SD	2.35	0.83
1:A:90:VAL:CG1	1:A:97:MET:HE2	2.06	0.83
1:A:255:HIS:CD2	1:A:339:MET:HE2	2.14	0.83
1:A:267:PHE:CD1	1:A:321:VAL:HG13	2.14	0.82
1:A:338[A]:MET:HE3	1:A:347:VAL:HG21	1.60	0.82
1:A:129:THR:HG22	1:A:215:ARG:HH11	1.45	0.81
1:A:184:ILE:HD11	1:A:188:LEU:CD1	2.10	0.81
1:A:35:LEU:CD2	1:A:44:LEU:HD13	2.11	0.81
1:A:33:LEU:HG	1:A:72:ALA:HB2	1.63	0.80
1:A:24:ARG:H	1:A:25:PRO:HD3	1.46	0.80
1:A:23:GLY:O	1:A:24:ARG:HB3	1.81	0.80
1:B:298:GLU:HB2	4:B:489:HOH:O	1.81	0.79
1:A:23:GLY:O	1:A:24:ARG:CB	2.30	0.77
1:B:187:SER:HB3	4:B:487:HOH:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLN:HG3	4:B:440:HOH:O	1.86	0.75
1:A:150:ALA:CA	1:A:152:ALA:H	1.97	0.74
1:A:278:PHE:HZ	4:A:389:HOH:O	1.71	0.73
1:A:267:PHE:CD1	1:A:321:VAL:HG12	2.16	0.73
1:A:92:LEU:HD21	4:A:433:HOH:O	1.87	0.73
1:B:204:MET:HE2	1:B:207:LEU:HD12	1.69	0.72
1:A:136:LYS:CD	1:A:204:MET:HE1	2.19	0.72
1:A:24:ARG:H	1:A:25:PRO:CD	2.01	0.72
1:A:136:LYS:HD2	1:A:204:MET:CE	2.20	0.71
1:B:215:ARG:HG2	1:B:215:ARG:NH1	1.95	0.71
1:B:204:MET:CE	1:B:204:MET:HA	2.20	0.71
1:A:315:MET:HE1	1:A:342:ASP:C	2.11	0.71
1:A:249:PRO:HD2	1:A:348:GLN:HE21	1.57	0.70
1:B:19:GLY:HA2	4:B:560:HOH:O	1.92	0.70
1:A:149:ALA:O	1:A:150:ALA:C	2.29	0.70
1:A:23:GLY:O	1:A:24:ARG:HG2	1.92	0.68
1:B:249:PRO:HD2	1:B:348:GLN:HE21	1.58	0.68
1:B:165:GLU:O	1:B:165:GLU:HG2	1.92	0.68
1:A:33:LEU:HG	1:A:72:ALA:CB	2.24	0.67
1:B:136:LYS:HA	1:B:204:MET:HE1	1.76	0.67
1:B:212:ASN:HB2	4:B:417:HOH:O	1.94	0.67
1:A:278:PHE:CZ	4:A:389:HOH:O	2.45	0.67
1:A:136:LYS:CD	1:A:204:MET:CE	2.73	0.66
1:A:184:ILE:CD1	1:A:188:LEU:HD11	2.15	0.66
1:A:35:LEU:HD22	1:A:44:LEU:HD13	1.78	0.66
1:B:332:LYS:CB	4:B:421:HOH:O	2.43	0.66
1:A:203:LEU:O	1:A:206:MET:HG2	1.97	0.65
1:A:118:ASN:HB3	1:A:119:LEU:C	2.17	0.64
1:A:296:ASN:HB2	1:A:297:PRO:CD	2.27	0.64
1:B:150:ALA:N	1:B:156:ASN:HD21	1.95	0.63
1:A:51:MET:HE1	1:A:198:LYS:HG3	1.80	0.62
1:A:255:HIS:CD2	1:A:339:MET:HE1	2.22	0.62
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.82	0.61
1:A:282:ARG:HD2	1:A:316:GLU:HG2	1.81	0.61
1:A:23:GLY:O	1:A:24:ARG:CG	2.49	0.60
1:B:146:MET:HE3	1:B:158:MET:N	2.16	0.60
1:B:273:LEU:HD13	1:B:302:ALA:HB2	1.83	0.59
1:A:155:LEU:HD11	1:A:241:PHE:CE1	2.37	0.59
1:B:12:LYS:HE3	1:B:230:PHE:CE2	2.37	0.59
1:A:150:ALA:CA	1:A:152:ALA:N	2.58	0.59
1:A:118:ASN:HB2	1:A:119:LEU:HA	1.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:O	1:A:49:LEU:HB2	2.02	0.59
1:B:118:ASN:C	1:B:118:ASN:HD22	2.07	0.57
1:B:217:GLN:NE2	1:B:224:ARG:HE	2.02	0.57
1:B:44:LEU:HD12	1:B:44:LEU:N	2.20	0.57
1:B:184:ILE:HG22	1:B:186:GLN:HB2	1.87	0.57
1:B:273:LEU:HD12	1:B:273:LEU:N	2.19	0.57
1:B:204:MET:CE	1:B:207:LEU:HD12	2.34	0.56
1:A:315:MET:HE1	1:A:342:ASP:HA	1.87	0.56
1:A:198:LYS:HG2	4:A:441:HOH:O	2.04	0.56
1:A:90:VAL:HG13	1:A:97:MET:CE	2.34	0.56
1:A:35:LEU:CD2	1:A:44:LEU:CD1	2.84	0.56
1:B:100:ARG:HG2	1:B:105:ARG:HG2	1.88	0.55
1:B:146:MET:HE3	1:B:157:GLY:C	2.26	0.55
1:A:278:PHE:C	1:A:278:PHE:CD2	2.80	0.55
1:A:315:MET:HE1	1:A:343:SER:N	2.22	0.55
1:B:204:MET:HA	1:B:204:MET:HE2	1.90	0.54
1:B:95:GLU:HG2	4:B:446:HOH:O	2.06	0.54
1:A:12:LYS:HG2	1:A:13:PRO:CD	2.28	0.53
1:A:206:MET:HG3	1:A:207:LEU:HD13	1.90	0.53
1:B:204:MET:HE3	1:B:204:MET:HA	1.91	0.53
1:A:27:LEU:HD12	1:A:28:PRO:HD2	1.91	0.52
1:B:214:LEU:CD1	1:B:227:VAL:HG22	2.40	0.52
1:B:129:THR:H	1:B:186:GLN:NE2	2.08	0.52
1:B:215:ARG:NH1	1:B:215:ARG:CG	2.72	0.52
1:A:315:MET:HE1	1:A:342:ASP:CA	2.39	0.52
1:B:129:THR:H	1:B:186:GLN:HE22	1.58	0.52
1:A:92:LEU:CD2	4:A:433:HOH:O	2.54	0.52
1:A:12:LYS:CG	1:A:13:PRO:HD3	2.29	0.51
1:B:332:LYS:HB2	4:B:421:HOH:O	2.07	0.51
1:A:214:LEU:HD13	1:A:227:VAL:HG22	1.92	0.51
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.92	0.51
1:A:320:ASN:HB2	1:A:364[A]:MET:HE3	1.93	0.51
1:B:35:LEU:HD11	1:B:70:VAL:HG22	1.93	0.51
1:A:149:ALA:O	1:A:150:ALA:O	2.29	0.50
1:B:258:ALA:HB3	1:B:263:LEU:HD21	1.94	0.50
1:B:130:LEU:HD21	1:B:214:LEU:HD23	1.93	0.50
1:B:170:VAL:HG21	1:B:244:TYR:CE1	2.47	0.50
1:B:146:MET:HE1	1:B:197:ARG:HA	1.94	0.49
1:B:198:LYS:O	1:B:202:GLU:HG2	2.12	0.49
1:A:12:LYS:HG3	1:A:230:PHE:HZ	1.78	0.49
1:A:244:TYR:HD2	4:A:440:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLN:HE22	1:A:208:ASP:HB2	1.78	0.48
1:B:35:LEU:HD12	1:B:35:LEU:N	2.29	0.48
1:B:70:VAL:HB	1:B:71:PRO:HD2	1.96	0.48
1:B:159:LEU:HD11	1:B:192:SER:OG	2.14	0.48
1:B:258:ALA:HB2	1:B:308:VAL:HG12	1.95	0.48
1:B:168:ARG:HD2	1:B:244:TYR:OH	2.14	0.47
1:A:278:PHE:CZ	1:A:364[A]:MET:HE2	2.50	0.47
1:B:252:PRO:HB2	1:B:339:MET:HB3	1.96	0.46
1:B:214:LEU:HD13	1:B:227:VAL:CG2	2.46	0.46
1:A:338[A]:MET:HB3	1:A:338[A]:MET:HE3	1.76	0.46
1:A:24:ARG:N	1:A:25:PRO:CD	2.69	0.45
1:B:138:LEU:CD1	1:B:167:LEU:HD13	2.46	0.45
1:A:130:LEU:H	1:A:130:LEU:HD23	1.81	0.45
1:B:283:LEU:O	1:B:316:GLU:HA	2.16	0.45
1:A:136:LYS:CD	1:A:204:MET:HE3	2.46	0.45
1:B:33:LEU:CD1	1:B:35:LEU:HD11	2.47	0.45
1:B:214:LEU:HD12	1:B:227:VAL:HG22	1.99	0.44
1:A:67:ALA:O	1:A:68:THR:HG22	2.17	0.44
1:A:14:LEU:O	1:A:18:SER:CB	2.66	0.44
1:A:257:GLU:HB2	1:A:309:THR:HB	2.00	0.44
1:B:217:GLN:HE22	1:B:224:ARG:HE	1.66	0.44
1:A:24:ARG:N	1:A:25:PRO:HD3	2.25	0.44
1:B:61:GLN:NE2	1:B:87:GLU:OE1	2.49	0.44
1:A:14:LEU:O	1:A:18:SER:HB2	2.17	0.43
1:A:214:LEU:CD1	1:A:227:VAL:HG22	2.48	0.43
1:A:296:ASN:HB2	1:A:297:PRO:HD3	2.00	0.43
1:A:130:LEU:N	1:A:130:LEU:HD23	2.33	0.43
1:A:159:LEU:HD11	1:A:192:SER:OG	2.18	0.43
1:B:77:ASP:OD1	1:B:80:ARG:NH2	2.50	0.43
1:A:315:MET:CE	1:A:342:ASP:HA	2.47	0.43
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.88	0.43
1:B:214:LEU:HD13	1:B:227:VAL:HG22	2.01	0.43
1:B:18:SER:HA	1:B:21:LEU:HD13	2.00	0.43
1:B:246:ARG:H	1:B:246:ARG:HG2	1.69	0.43
1:B:214:LEU:CD1	1:B:227:VAL:CG2	2.97	0.43
1:A:300:GLU:HG2	1:B:108:LEU:HA	2.01	0.42
1:A:137:ARG:CZ	4:A:429:HOH:O	2.67	0.42
1:B:258:ALA:HB3	1:B:263:LEU:CD2	2.49	0.42
1:A:152:ALA:O	1:A:153:TYR:O	2.38	0.41
1:A:285:VAL:HG11	1:A:310:TYR:CD1	2.55	0.41
1:B:281:VAL:HG12	1:B:294:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLU:HA	1:B:65:PRO:HD3	1.88	0.41
1:B:165:GLU:O	1:B:165:GLU:CG	2.63	0.41
1:A:19:GLY:O	1:A:205:ARG:CZ	2.68	0.41
1:A:237:VAL:HG11	4:A:479:HOH:O	2.20	0.40
1:A:264:LYS:HD3	4:A:425:HOH:O	2.20	0.40
1:A:1:MET:HE2	1:A:67:ALA:N	2.36	0.40
1:B:12:LYS:HE3	1:B:230:PHE:CZ	2.56	0.40
1:B:226[A]:HIS:CD2	1:B:231:ILE:HG23	2.57	0.40
1:B:21:LEU:CD2	1:B:72:ALA:HB3	2.51	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
4:A:420:HOH:O	4:B:573:HOH:O[1_545]	1.74	0.46
4:B:376:HOH:O	4:B:555:HOH:O[1_455]	1.97	0.23

## 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	364/366 (100%)	347 (95%)	8 (2%)	9 (2%)	6	1
1	B	364/366 (100%)	352 (97%)	12 (3%)	0	100	100
All	All	728/732 (100%)	699 (96%)	20 (3%)	9 (1%)	15	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	24	ARG
1	A	68	THR

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Mol	Chain	Res	Type
1	A	153	TYR
1	A	212	ASN
1	A	118	ASN
1	A	39[A]	ASP
1	A	25	PRO
1	A	150	ALA

### 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	308/308 (100%)	278 (90%)	30 (10%)	9	2
1	B	308/308 (100%)	290 (94%)	18 (6%)	23	8
All	All	616/616 (100%)	568 (92%)	48 (8%)	15	4

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	20	PRO
1	A	26	THR
1	A	44	LEU
1	A	52	GLU
1	A	57	VAL
1	A	92	LEU
1	A	98	LEU
1	A	119	LEU
1	A	129	THR
1	A	155	LEU
1	A	176	ARG
1	A	187	SER
1	A	188	LEU
1	A	203	LEU
1	A	207	LEU
1	A	212	ASN

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Mol	Chain	Res	Type
1	A	226	HIS
1	A	227	VAL
1	A	238	ASP
1	A	240	ARG
1	A	256	LEU
1	A	264	LYS
1	A	278	PHE
1	A	282	ARG
1	A	315	MET
1	A	321	VAL
1	A	338[A]	MET
1	A	339	MET
1	A	365	ARG
1	B	16	GLN
1	B	118	ASN
1	B	137	ARG
1	B	167	LEU
1	B	168	ARG
1	B	176	ARG
1	B	191	HIS
1	B	203	LEU
1	B	204	MET
1	B	212	ASN
1	B	215	ARG
1	B	246	ARG
1	B	247	VAL
1	B	255	HIS
1	B	263	LEU
1	B	311	SER
1	B	332	LYS
1	B	366	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	A	251	ASN
1	A	255	HIS
1	A	288	ASN
1	A	329	ASN
1	A	335	ASN
1	A	348	GLN

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Mol	Chain	Res	Type
1	B	156	ASN
1	B	186	GLN
1	B	212	ASN
1	B	217	GLN
1	B	226[A]	HIS
1	B	255	HIS
1	B	329	ASN
1	B	348	GLN

### 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	366/366 (100%)	0.34	24 (6%)	19 19	21, 33, 51, 76	1 (0%)
1	B	366/366 (100%)	0.35	17 (4%)	33 32	22, 33, 54, 63	2 (0%)
All	All	732/732 (100%)	0.34	41 (5%)	25 24	21, 33, 51, 76	3 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	GLY	9.7
1	B	21	LEU	9.2
1	B	153	TYR	6.0
1	A	26	THR	5.7
1	B	366	LEU	5.6
1	A	27	LEU	5.6
1	B	23	GLY	5.3
1	B	209	GLY	5.1
1	A	150	ALA	5.1
1	A	22	GLY	4.9
1	A	278	PHE	4.6
1	A	24	ARG	4.5
1	A	20	PRO	4.0
1	A	366	LEU	3.9
1	B	252	PRO	3.6
1	B	211	ASP	3.5
1	A	182[A]	MET	3.4
1	A	152	ALA	3.3
1	A	23	GLY	3.2
1	A	118	ASN	3.1
1	A	19	GLY	2.9
1	B	17	VAL	2.9
1	A	49	LEU	2.8
1	B	243	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	210	GLY	2.7
1	B	20	PRO	2.6
1	A	239	GLY	2.6
1	A	240	ARG	2.5
1	A	25	PRO	2.4
1	A	67	ALA	2.4
1	B	247	VAL	2.3
1	A	21	LEU	2.3
1	A	365	ARG	2.3
1	B	151	ALA	2.3
1	A	247	VAL	2.3
1	B	148	ALA	2.2
1	B	251	ASN	2.2
1	B	208	ASP	2.2
1	A	250	LYS	2.2
1	A	238	ASP	2.1
1	A	347	VAL	2.1

## 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	B	368	1/1	0.97	0.17	2.27	30,30,30,30	0
2	CA	B	367	1/1	1.00	0.01	-2.24	29,29,29,29	0
2	CA	A	367	1/1	1.00	0.03	-2.35	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.