



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:01 PM UTC

PDB ID : 2Y1R / pdb_00002y1r
Title : Structure of MecA121 & ClpC N-domain complex
Authors : Wang, F.; Mei, Z.Q.; Wang, J.W.; Shi, Y.G.
Deposited on : 2010-12-10
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

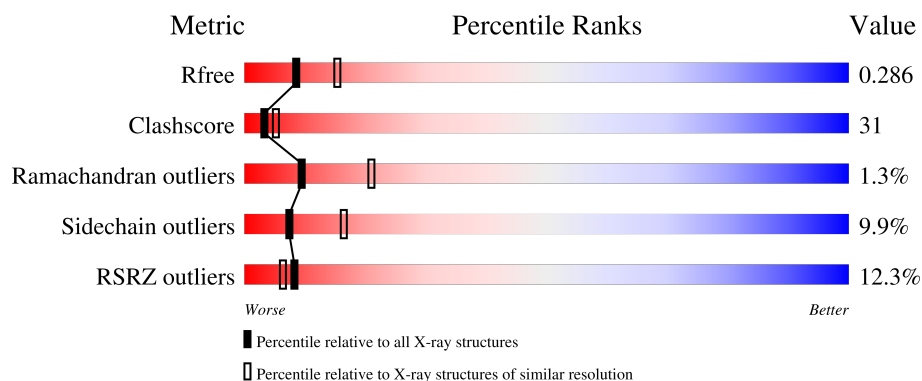
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 ≥ 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	149	16% 50% 34% 9% 6%
1	B	149	13% 50% 32% 10% 7%
1	C	149	11% 50% 34% 9% 7%
1	D	149	11% 49% 38% 8% 5%
1	E	149	13% 51% 33% 9% 7%

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Mol	Chain	Length	Quality of chain
1	F	149	
1	G	149	
1	H	149	
2	I	98	
2	J	98	
2	K	98	
2	L	98	
2	M	98	
2	N	98	
2	O	98	
2	P	98	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14113 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 NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1070	667	202	199	2			
1	B	139	Total	C	N	O	S	0	0	0
			1065	664	201	198	2			
1	C	139	Total	C	N	O	S	0	0	0
			1065	664	201	198	2			
1	D	141	Total	C	N	O	S	0	0	0
			1074	669	203	200	2			
1	E	139	Total	C	N	O	S	0	0	0
			1065	664	201	198	2			
1	F	133	Total	C	N	O	S	0	0	0
			1019	639	191	188	1			
1	G	139	Total	C	N	O	S	0	0	0
			1065	664	201	198	2			
1	H	139	Total	C	N	O	S	0	0	0
			1065	664	201	198	2			

- Molecule 2 is a protein called ADAPTER PROTEIN MECA 1.

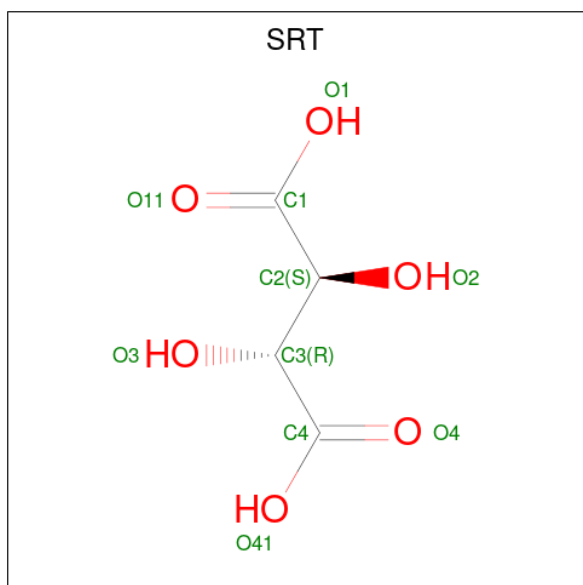
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			
2	J	95	Total	C	N	O	S	0	0	0
			785	503	124	156	2			
2	K	92	Total	C	N	O	S	0	0	0
			757	487	119	149	2			
2	L	4	Total	C	N	O		0	0	0
			32	21	6	5				
2	M	90	Total	C	N	O	S	0	0	0
			742	478	116	146	2			
2	N	89	Total	C	N	O	S	0	0	0
			742	480	116	144	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	89	Total	C	N	O	S	0	0	0
			739	478	115	144	2			
2	P	94	Total	C	N	O	S	0	0	0
			776	498	123	153	2			

- Molecule 3 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	E	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 10 4 6	0	0
3	F	1	Total C O 10 4 6	0	0
3	F	1	Total C O 10 4 6	0	0
3	G	1	Total C O 10 4 6	0	0
3	G	1	Total C O 10 4 6	0	0
3	H	1	Total C O 10 4 6	0	0
3	H	1	Total C O 10 4 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	15	Total O 15 15	0	0
4	C	12	Total O 12 12	0	0
4	D	17	Total O 17 17	0	0
4	E	7	Total O 7 7	0	0
4	F	3	Total O 3 3	0	0
4	G	11	Total O 11 11	0	0
4	H	8	Total O 8 8	0	0
4	I	5	Total O 5 5	0	0
4	J	4	Total O 4 4	0	0
4	K	6	Total O 6 6	0	0
4	L	1	Total O 1 1	0	0

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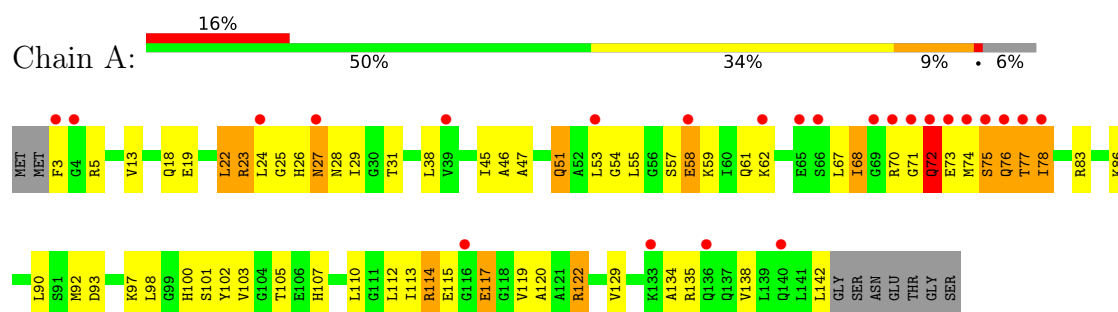
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	5	Total 5	O 5	0	0
4	N	5	Total 5	O 5	0	0
4	O	4	Total 4	O 4	0	0
4	P	3	Total 3	O 3	0	0

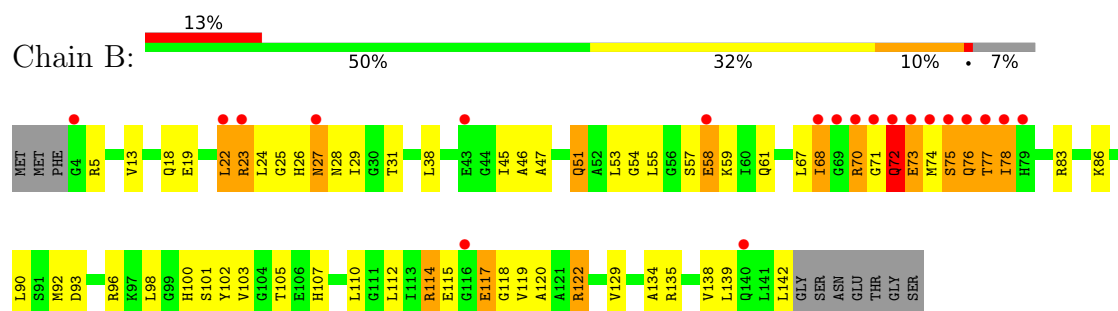
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

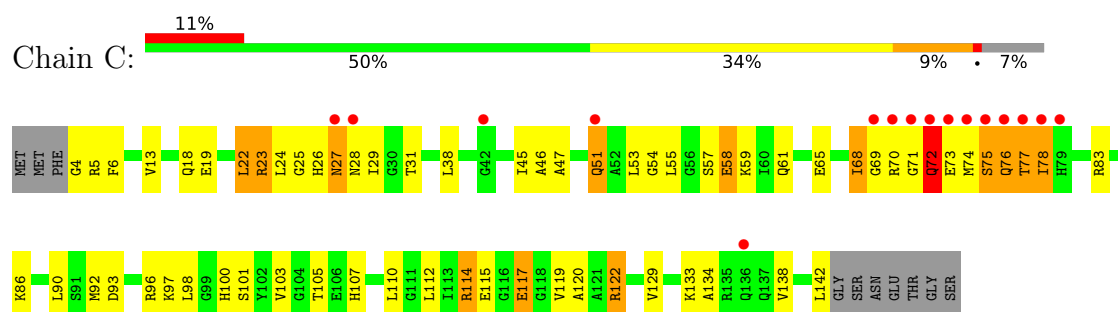
• Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB



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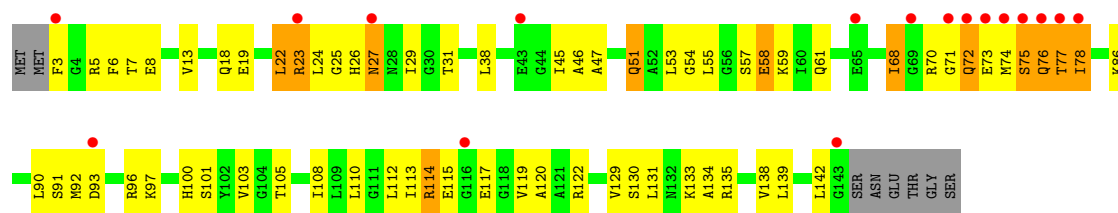


• Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

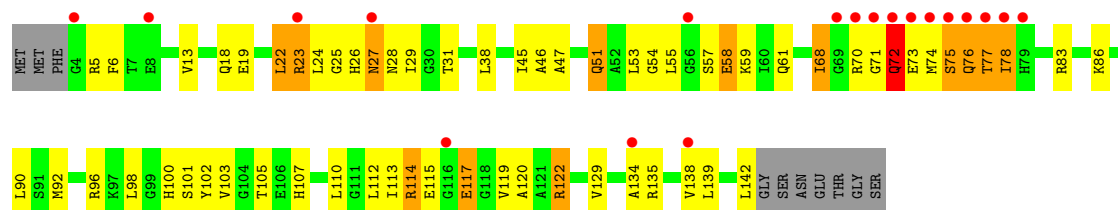


• Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

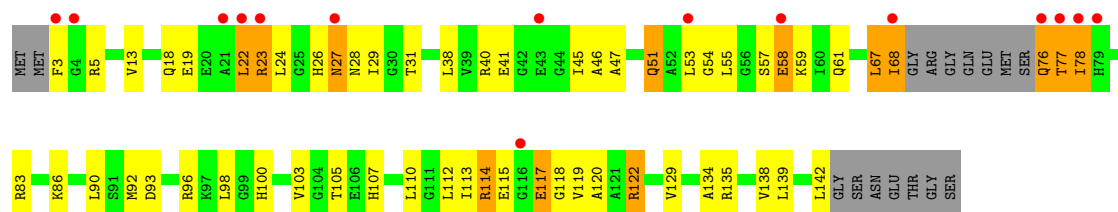




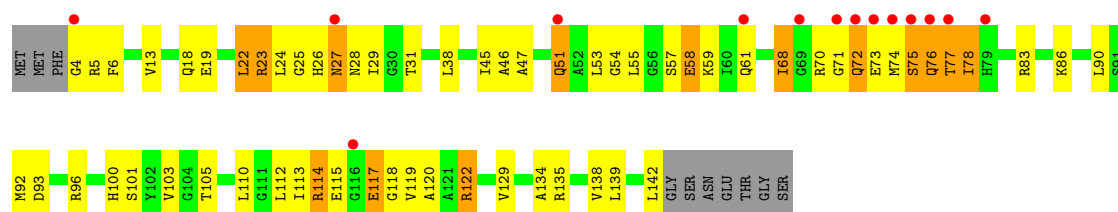
- Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB



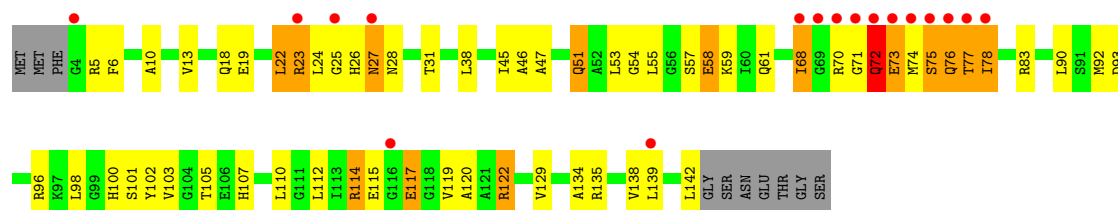
- Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB



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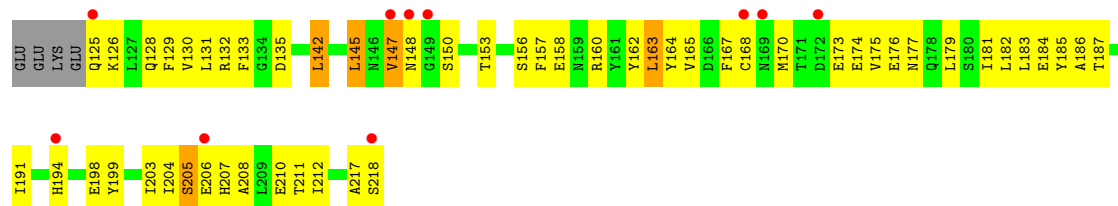


- Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB



- Molecule 2: ADAPTER PROTEIN MECA 1

Chain I: 



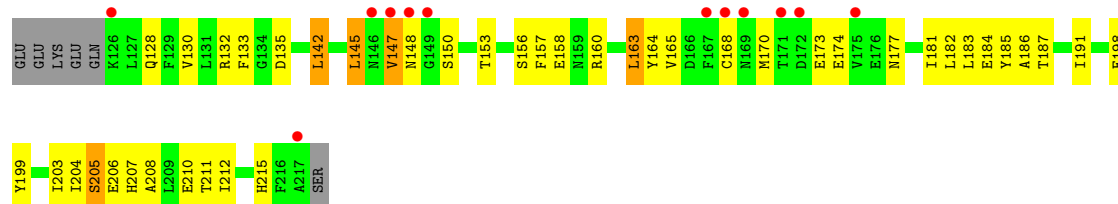
- Molecule 2: ADAPTER PROTEIN MECA 1

Chain J: 



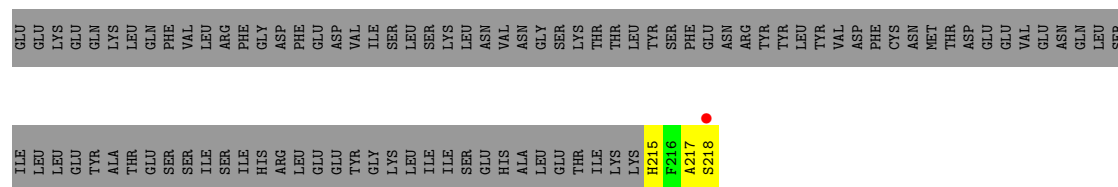
- Molecule 2: ADAPTER PROTEIN MECA 1

Chain K: 



- Molecule 2: ADAPTER PROTEIN MECA 1

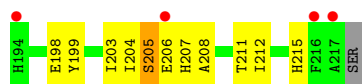
Chain L: 



- Molecule 2: ADAPTER PROTEIN MECA 1

Chain M: 





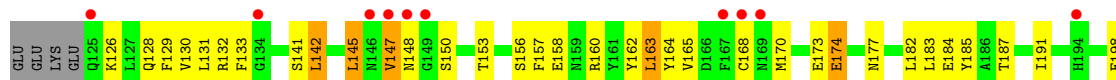
• Molecule 2: ADAPTER PROTEIN MECA 1



• Molecule 2: ADAPTER PROTEIN MECA 1



• Molecule 2: ADAPTER PROTEIN MECA 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.02Å 124.72Å 149.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.60 47.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (47.93-2.60) 94.1 (47.93-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.58Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.258 0.248 , 0.286	Depositor DCC
R_{free} test set	2915 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.358	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14113	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5401e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SRT

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	0.68	0/1078	0.94	1/1445 (0.1%)
1	B	0.68	0/1073	0.90	0/1438
1	C	0.65	0/1073	0.90	1/1438 (0.1%)
1	D	0.63	0/1082	0.93	1/1450 (0.1%)
1	E	0.59	0/1073	0.90	0/1438
1	F	0.63	0/1026	0.91	0/1376
1	G	0.62	0/1073	0.91	0/1438
1	H	1.47	1/1073 (0.1%)	0.94	0/1438
2	I	0.67	0/786	0.83	0/1059
2	J	0.66	0/799	0.83	1/1076 (0.1%)
2	K	0.57	0/771	0.79	0/1040
2	L	0.39	0/33	0.81	0/43
2	M	0.57	0/755	0.79	0/1016
2	N	0.61	0/755	0.83	0/1015
2	O	0.57	0/752	0.79	0/1013
2	P	0.59	0/790	0.78	0/1064
All	All	0.73	1/13992 (0.0%)	0.87	4/18787 (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
1	B	0	1
2	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	73	GLU	C-N	44.40	1.83	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	125	GLN	N-CA-C	6.62	120.45	109.46
1	A	101	SER	N-CA-C	-5.53	106.53	113.72
1	D	29	ILE	CB-CA-C	-5.28	106.20	111.80
1	C	133	LYS	N-CA-C	-5.06	105.84	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	ARG	Peptide
2	I	125	GLN	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	1070	0	1118	91	1
1	B	1065	0	1116	132	0
1	C	1065	0	1116	69	0
1	D	1074	0	1121	70	0
1	E	1065	0	1116	96	0
1	F	1019	0	1070	118	0
1	G	1065	0	1116	77	0
1	H	1065	0	1115	76	0
2	I	772	0	752	50	4
2	J	785	0	764	50	1
2	K	757	0	734	38	0
2	L	32	0	25	5	0
2	M	742	0	718	44	0
2	N	742	0	725	52	4
2	O	739	0	719	45	0
2	P	776	0	758	46	0
3	A	20	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	8	1	0
3	C	20	0	8	1	0
3	D	20	0	8	1	0
3	E	20	0	8	1	0
3	F	20	0	8	1	0
3	G	20	0	8	2	0
3	H	20	0	8	1	0
4	A	14	0	0	2	0
4	B	15	0	0	0	0
4	C	12	0	0	3	0
4	D	17	0	0	4	0
4	E	7	0	0	1	0
4	F	3	0	0	0	0
4	G	11	0	0	1	0
4	H	8	0	0	0	0
4	I	5	0	0	1	0
4	J	4	0	0	0	0
4	K	6	0	0	1	0
4	L	1	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	1	0
4	O	4	0	0	0	0
4	P	3	0	0	0	0
All	All	14113	0	14147	862	5

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 31.

The worst 5 of 862 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:B:73:GLU:CB	1:F:23:ARG:HG2	1.41	1.47
1:H:73:GLU:C	1:H:74:MET:N	1.83	1.35
1:B:73:GLU:HB2	1:F:23:ARG:CG	1.71	1.21
1:B:74:MET:N	1:F:23:ARG:HE	1.42	1.18
1:B:73:GLU:CD	1:F:24:LEU:HA	1.69	1.17

All (5) 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)
2:I:194:HIS:CE1	2:N:170:MET:O[2_455]	1.92	0.28
2:I:194:HIS:NE2	2:N:170:MET:O[2_455]	1.93	0.27
2:I:164:TYR:OH	2:N:174:GLU:OE2[2_455]	1.97	0.23
2:I:194:HIS:ND1	2:N:170:MET:N[2_455]	2.00	0.20
1:A:62:LYS:NZ	2:J:172:ASP:OD1[2_455]	2.12	0.08

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	138/149 (93%)	130 (94%)	5 (4%)	3 (2%)	5	10
1	B	137/149 (92%)	131 (96%)	3 (2%)	3 (2%)	5	10
1	C	137/149 (92%)	129 (94%)	5 (4%)	3 (2%)	5	10
1	D	139/149 (93%)	131 (94%)	5 (4%)	3 (2%)	5	10
1	E	137/149 (92%)	129 (94%)	5 (4%)	3 (2%)	5	10
1	F	129/149 (87%)	128 (99%)	0	1 (1%)	16	34
1	G	137/149 (92%)	129 (94%)	5 (4%)	3 (2%)	5	10
1	H	137/149 (92%)	129 (94%)	5 (4%)	3 (2%)	5	10
2	I	92/98 (94%)	88 (96%)	4 (4%)	0	100	100
2	J	93/98 (95%)	89 (96%)	4 (4%)	0	100	100
2	K	90/98 (92%)	84 (93%)	6 (7%)	0	100	100
2	L	2/98 (2%)	2 (100%)	0	0	100	100
2	M	86/98 (88%)	84 (98%)	2 (2%)	0	100	100
2	N	85/98 (87%)	82 (96%)	3 (4%)	0	100	100
2	O	85/98 (87%)	83 (98%)	2 (2%)	0	100	100
2	P	92/98 (94%)	88 (96%)	4 (4%)	0	100	100
All	All	1716/1976 (87%)	1636 (95%)	58 (3%)	22 (1%)	9	21

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	SER
1	A	75	SER
1	C	72	GLN
1	C	75	SER
1	D	75	SER

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	110/118 (93%)	98 (89%)	12 (11%)	6	13
1	B	110/118 (93%)	97 (88%)	13 (12%)	5	10
1	C	110/118 (93%)	98 (89%)	12 (11%)	6	13
1	D	110/118 (93%)	98 (89%)	12 (11%)	6	13
1	E	110/118 (93%)	98 (89%)	12 (11%)	6	13
1	F	105/118 (89%)	93 (89%)	12 (11%)	5	11
1	G	110/118 (93%)	98 (89%)	12 (11%)	6	13
1	H	110/118 (93%)	98 (89%)	12 (11%)	6	13
2	I	87/92 (95%)	80 (92%)	7 (8%)	11	25
2	J	89/92 (97%)	81 (91%)	8 (9%)	9	20
2	K	85/92 (92%)	78 (92%)	7 (8%)	10	24
2	L	3/92 (3%)	3 (100%)	0	100	100
2	M	83/92 (90%)	77 (93%)	6 (7%)	13	30
2	N	83/92 (90%)	77 (93%)	6 (7%)	13	30
2	O	83/92 (90%)	76 (92%)	7 (8%)	10	23
2	P	88/92 (96%)	80 (91%)	8 (9%)	9	19
All	All	1476/1680 (88%)	1330 (90%)	146 (10%)	7	16

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	163	LEU

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Mol	Chain	Res	Type
2	P	173	GLU
2	M	142	LEU
2	N	205	SER
1	D	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	125	ASN
2	N	207	HIS
1	G	27	ASN
2	N	125	GLN
2	P	207	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SRT	E	500	-	9,9,9	1.41	1 (11%)	12,12,12	1.39	2 (16%)
3	SRT	D	500	-	9,9,9	1.36	1 (11%)	12,12,12	1.54	3 (25%)
3	SRT	D	600	-	9,9,9	1.29	1 (11%)	12,12,12	1.30	2 (16%)
3	SRT	F	600	-	9,9,9	1.30	0	12,12,12	1.26	1 (8%)
3	SRT	A	600	-	9,9,9	1.36	1 (11%)	12,12,12	1.37	1 (8%)
3	SRT	A	500	-	9,9,9	1.38	1 (11%)	12,12,12	1.45	2 (16%)
3	SRT	B	500	-	9,9,9	1.34	1 (11%)	12,12,12	1.28	1 (8%)
3	SRT	G	500	-	9,9,9	1.41	1 (11%)	12,12,12	1.52	3 (25%)
3	SRT	H	600	-	9,9,9	1.25	0	12,12,12	1.32	2 (16%)
3	SRT	C	600	-	9,9,9	1.19	0	12,12,12	1.23	2 (16%)
3	SRT	G	600	-	9,9,9	1.37	1 (11%)	12,12,12	1.14	0
3	SRT	B	600	-	9,9,9	1.29	0	12,12,12	1.26	1 (8%)
3	SRT	C	500	-	9,9,9	1.27	0	12,12,12	1.39	1 (8%)
3	SRT	F	500	-	9,9,9	1.32	1 (11%)	12,12,12	1.38	1 (8%)
3	SRT	E	600	-	9,9,9	1.35	2 (22%)	12,12,12	1.27	1 (8%)
3	SRT	H	500	-	9,9,9	1.35	1 (11%)	12,12,12	1.43	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SRT	E	500	-	-	9/12/12/12	-
3	SRT	D	500	-	-	9/12/12/12	-
3	SRT	D	600	-	-	9/12/12/12	-
3	SRT	F	600	-	-	9/12/12/12	-
3	SRT	A	600	-	-	9/12/12/12	-
3	SRT	A	500	-	-	9/12/12/12	-
3	SRT	B	500	-	-	9/12/12/12	-
3	SRT	G	500	-	-	9/12/12/12	-
3	SRT	H	600	-	-	8/12/12/12	-
3	SRT	C	600	-	-	9/12/12/12	-
3	SRT	G	600	-	-	9/12/12/12	-
3	SRT	B	600	-	-	9/12/12/12	-
3	SRT	C	500	-	-	9/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SRT	F	500	-	-	9/12/12/12	-
3	SRT	E	600	-	-	9/12/12/12	-
3	SRT	H	500	-	-	9/12/12/12	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	SRT	C2-C1	-2.65	1.48	1.52
3	G	500	SRT	C3-C4	-2.47	1.49	1.52
3	D	500	SRT	C3-C4	-2.46	1.49	1.52
3	E	500	SRT	C3-C4	-2.43	1.49	1.52
3	A	500	SRT	C3-C4	-2.19	1.49	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	500	SRT	C2-C3-C4	-3.10	102.95	109.82
3	A	500	SRT	C2-C3-C4	-2.87	103.45	109.82
3	G	500	SRT	C2-C3-C4	-2.86	103.47	109.82
3	H	500	SRT	C2-C3-C4	-2.74	103.74	109.82
3	F	500	SRT	C2-C3-C4	-2.74	103.74	109.82

There are no chirality outliers.

5 of 143 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	SRT	O1-C1-C2-O2
3	A	500	SRT	O1-C1-C2-C3
3	A	500	SRT	O11-C1-C2-O2
3	A	500	SRT	O11-C1-C2-C3
3	B	500	SRT	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	600	SRT	1	0
3	F	600	SRT	1	0
3	A	600	SRT	1	0
3	H	600	SRT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	600	SRT	1	0
3	G	600	SRT	2	0
3	B	600	SRT	1	0
3	E	600	SRT	1	0

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
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	73:GLU	C	74:MET	N	1.83

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, 95th 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 ²)	Q<0.9
1	A	140/149 (93%)	1.05	24 (17%) 4 3	29, 48, 131, 407	0
1	B	139/149 (93%)	0.83	20 (14%) 6 5	29, 47, 134, 410	0
1	C	139/149 (93%)	0.85	16 (11%) 9 7	31, 49, 120, 404	0
1	D	141/149 (94%)	0.81	17 (12%) 8 6	30, 49, 106, 403	0
1	E	139/149 (93%)	0.85	19 (13%) 6 5	31, 49, 121, 406	0
1	F	133/149 (89%)	0.69	15 (11%) 10 8	32, 49, 84, 139	0
1	G	139/149 (93%)	0.76	14 (10%) 12 9	31, 48, 119, 406	0
1	H	139/149 (93%)	0.76	17 (12%) 8 6	32, 51, 115, 408	0
2	I	94/98 (95%)	0.75	10 (10%) 11 9	31, 48, 96, 129	0
2	J	95/98 (96%)	0.78	10 (10%) 11 9	31, 46, 98, 129	0
2	K	92/98 (93%)	0.87	12 (13%) 7 5	33, 49, 101, 131	0
2	L	4/98 (4%)	1.07	1 (25%) 2 1	40, 47, 59, 82	0
2	M	90/98 (91%)	0.74	12 (13%) 7 5	36, 51, 85, 109	0
2	N	89/98 (90%)	0.53	5 (5%) 30 24	31, 47, 79, 104	0
2	O	89/98 (90%)	0.89	13 (14%) 6 4	31, 51, 86, 129	0
2	P	94/98 (95%)	0.80	11 (11%) 9 7	34, 48, 99, 140	0
All	All	1756/1976 (88%)	0.80	216 (12%) 8 6	29, 49, 103, 410	0

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	GLY	7.1
1	H	73	GLU	6.9
1	A	73	GLU	6.8
2	O	147	VAL	6.5
1	A	69	GLY	6.4

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 oligosaccharides 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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
3	SRT	C	500	10/10	0.78	0.17	71,83,100,112	0
3	SRT	A	600	10/10	0.79	0.16	49,60,76,77	0
3	SRT	G	500	10/10	0.80	0.16	69,82,99,109	0
3	SRT	H	600	10/10	0.81	0.17	44,67,85,86	0
3	SRT	D	500	10/10	0.82	0.16	75,84,102,108	0
3	SRT	F	500	10/10	0.83	0.14	73,81,97,110	0
3	SRT	A	500	10/10	0.84	0.15	59,83,92,105	0
3	SRT	H	500	10/10	0.85	0.14	73,83,99,104	0
3	SRT	G	600	10/10	0.87	0.15	44,61,75,85	0
3	SRT	B	500	10/10	0.87	0.15	58,76,96,104	0
3	SRT	E	500	10/10	0.87	0.13	74,83,96,108	0
3	SRT	D	600	10/10	0.89	0.10	53,68,75,81	0
3	SRT	B	600	10/10	0.90	0.13	41,64,76,76	0
3	SRT	E	600	10/10	0.90	0.11	48,63,74,81	0
3	SRT	C	600	10/10	0.90	0.12	37,62,75,78	0
3	SRT	F	600	10/10	0.90	0.13	42,66,81,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.