



wwPDB X-ray Structure Validation Summary Report

Nov 20, 2014 – 10:02 PM EST

PDB ID : 2Y1R
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 validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

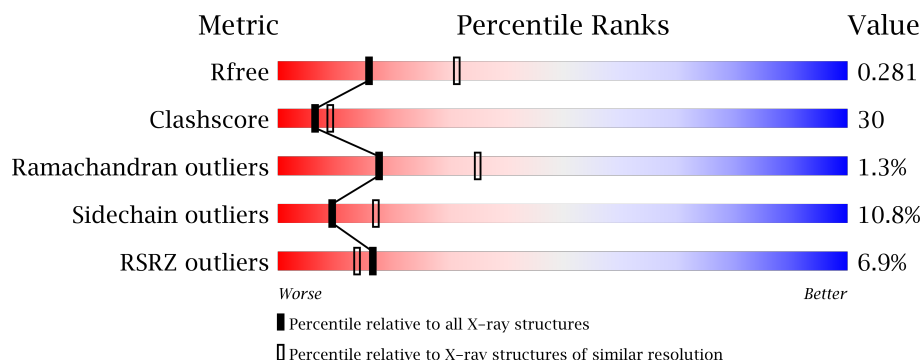
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24195
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	149	
1	B	149	
1	C	149	
1	D	149	
1	E	149	
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	

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Mol	Chain	Length	Quality of chain
2	O	98	
2	P	98	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SRT	A	500	-	X
3	SRT	C	500	-	X
3	SRT	G	500	-	X
3	SRT	H	600	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14113 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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.

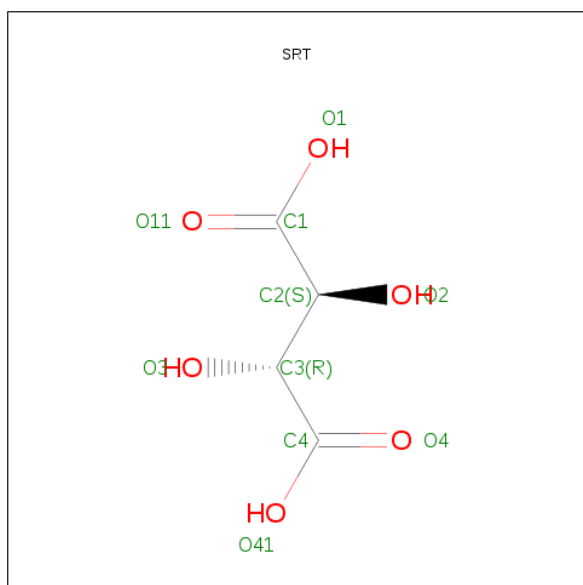
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			
2	J	95	Total	C	N	O	S	0	0	0
			785	503	124	156	2			
2	K	92	Total	C	N	O	S	0	0	0
			757	487	119	149	2			
2	L	4	Total	C	N	O		0	0	0
			32	21	6	5				
2	M	90	Total	C	N	O	S	0	0	0
			742	478	116	146	2			
2	N	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 (three-letter code: 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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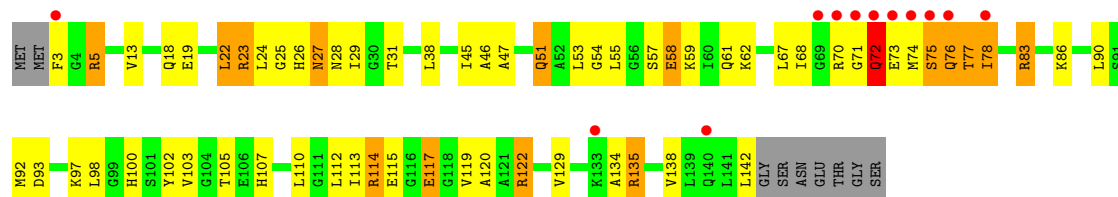
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	5	Total 5	O 5	0	0
4	N	5	Total 5	O 5	0	0
4	O	4	Total 4	O 4	0	0
4	P	3	Total 3	O 3	0	0

3 Residue-property plots

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.

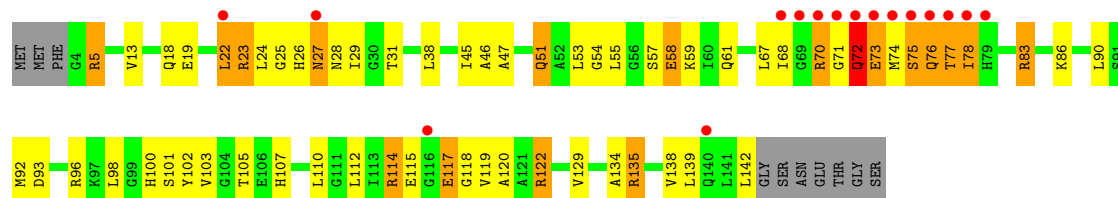
• Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

Chain A: 



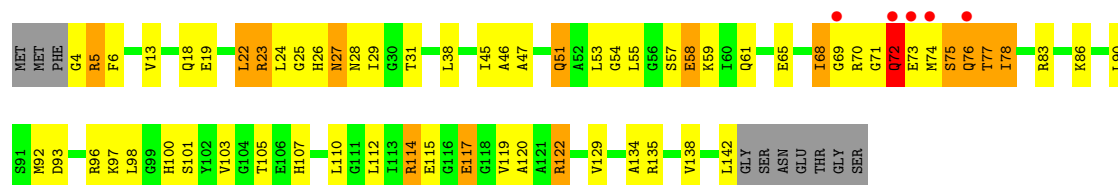
• Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

Chain B: 



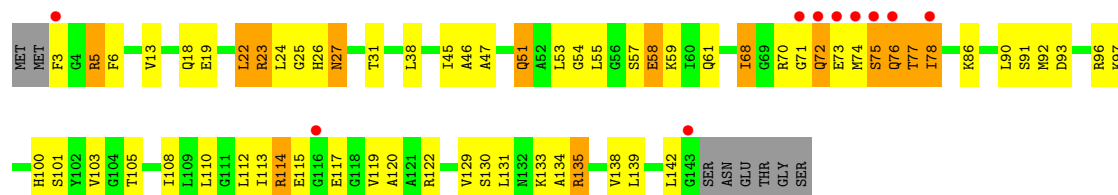
• Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

Chain C: 



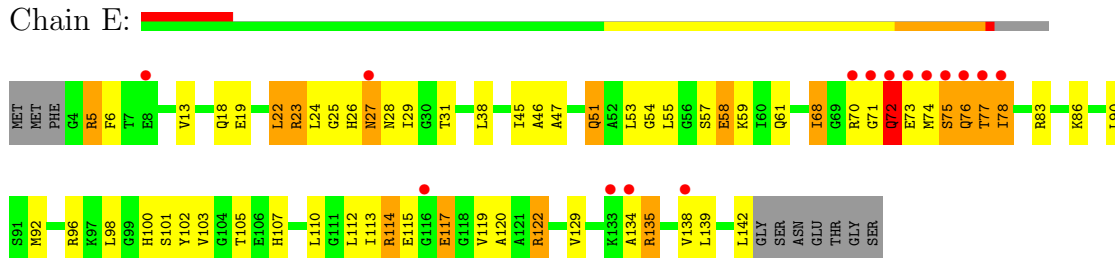
• Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

Chain D: 



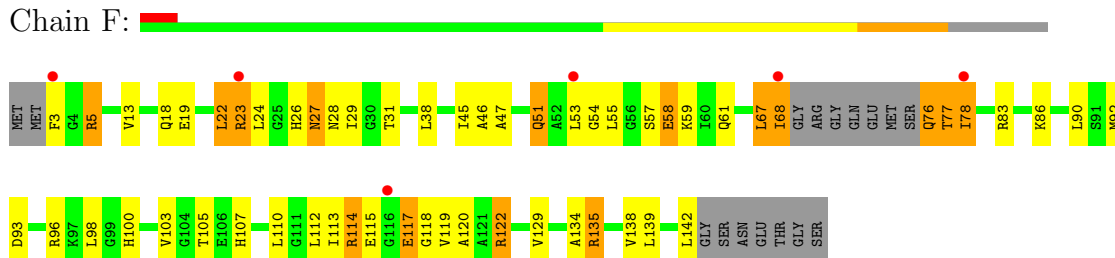
- Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

Chain E:



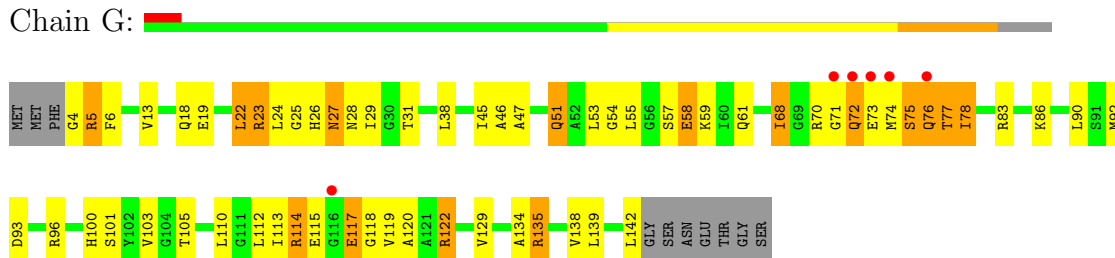
- Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

Chain F:



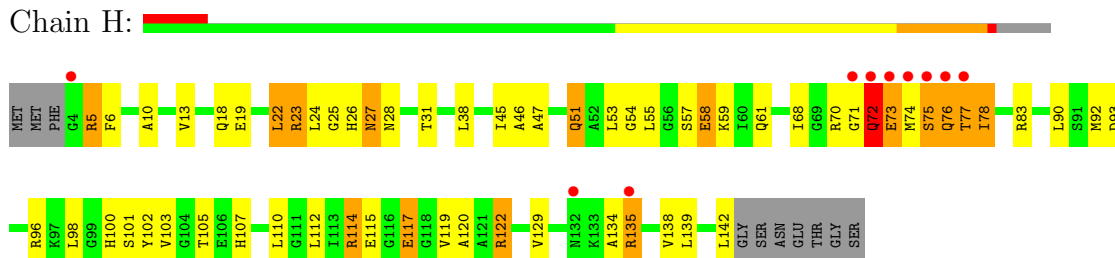
- Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

Chain G:



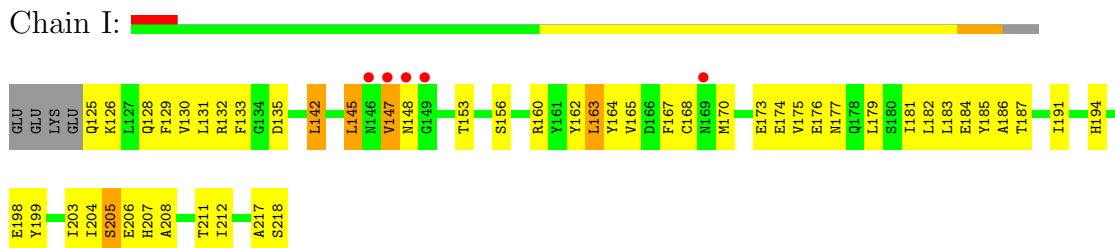
- Molecule 1: NEGATIVE REGULATOR OF GENETIC COMPETENCE CLPC/MECB

Chain H:



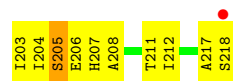
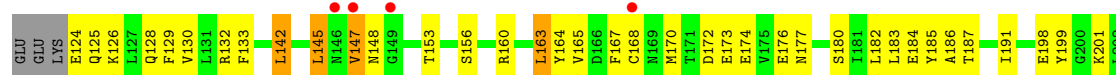
- Molecule 2: ADAPTER PROTEIN MECA 1

Chain I:



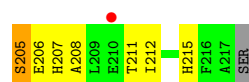
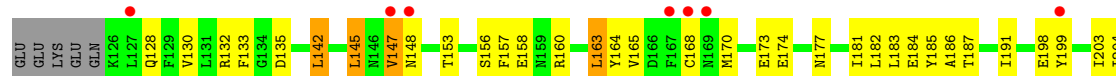
- Molecule 2: ADAPTER PROTEIN MECA 1

Chain J:



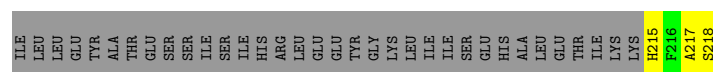
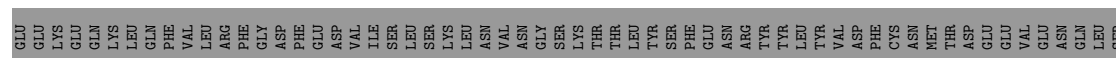
• Molecule 2: ADAPTER PROTEIN MECA 1

Chain K:



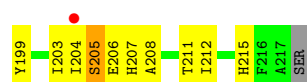
• Molecule 2: ADAPTER PROTEIN MECA 1

Chain L:



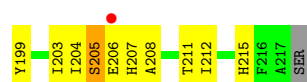
• Molecule 2: ADAPTER PROTEIN MECA 1

Chain M:



• Molecule 2: ADAPTER PROTEIN MECA 1

Chain N:



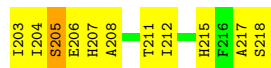
• Molecule 2: ADAPTER PROTEIN MECA 1

Chain O:



● Molecule 2: ADAPTER PROTEIN MECA 1

Chain P:



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 – 2.59	Depositor EDS
% Data completeness (in resolution range)	94.1 (47.93-2.60) 94.2 (47.93-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.258 0.235 , 0.281	Depositor DCC
R_{free} test set	2915 reflections (4.81%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 60654 reflections (0.003%)	Xtriage
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

Xtriage'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.

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	0.48	0/1078	0.66	1/1445 (0.1%)
1	B	0.49	0/1073	0.63	1/1438 (0.1%)
1	C	0.46	0/1073	0.61	0/1438
1	D	0.45	0/1082	0.62	0/1450
1	E	0.43	0/1073	0.61	0/1438
1	F	0.46	0/1026	0.64	0/1376
1	G	0.44	0/1073	0.62	0/1438
1	H	0.79	1/1073 (0.1%)	0.64	0/1438
2	I	0.54	0/786	0.61	0/1059
2	J	0.53	0/799	0.61	0/1076
2	K	0.48	0/771	0.58	0/1040
2	L	0.44	0/33	0.68	0/43
2	M	0.48	0/755	0.59	0/1016
2	N	0.48	0/755	0.60	0/1015
2	O	0.49	0/752	0.60	0/1013
2	P	0.48	0/790	0.57	0/1064
All	All	0.51	1/13992 (0.0%)	0.61	2/18787 (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	21.52	1.83	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	B	83	ARG	NE-CZ-NH1	-5.93	117.33	120.30

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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1070	0	1118	89	1
1	B	1065	0	1116	129	0
1	C	1065	0	1116	68	0
1	D	1074	0	1121	68	0
1	E	1065	0	1116	93	0
1	F	1019	0	1070	115	0
1	G	1065	0	1116	76	0
1	H	1065	0	1115	75	0
2	I	772	0	752	47	4
2	J	785	0	764	47	1
2	K	757	0	734	36	0
2	L	32	0	25	5	0
2	M	742	0	718	42	0
2	N	742	0	725	52	4
2	O	739	0	719	44	0
2	P	776	0	758	44	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	836	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

The worst 5 of 836 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	1.30
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:CB	1:F:23:ARG:CG	2.22	1.16

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	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	138/149 (93%)	130 (94%)	5 (4%)	3 (2%)	10	18
1	B	137/149 (92%)	131 (96%)	3 (2%)	3 (2%)	10	18
1	C	137/149 (92%)	129 (94%)	5 (4%)	3 (2%)	10	18
1	D	139/149 (93%)	131 (94%)	5 (4%)	3 (2%)	10	18
1	E	137/149 (92%)	129 (94%)	5 (4%)	3 (2%)	10	18
1	F	129/149 (87%)	128 (99%)	0	1 (1%)	27	53
1	G	137/149 (92%)	129 (94%)	5 (4%)	3 (2%)	10	18
1	H	137/149 (92%)	129 (94%)	5 (4%)	3 (2%)	10	18
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%)	18	35

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%)	97 (88%)	13 (12%)	8	14
1	B	110/118 (93%)	96 (87%)	14 (13%)	6	12
1	C	110/118 (93%)	96 (87%)	14 (13%)	6	12
1	D	110/118 (93%)	96 (87%)	14 (13%)	6	12
1	E	110/118 (93%)	96 (87%)	14 (13%)	6	12
1	F	105/118 (89%)	91 (87%)	14 (13%)	6	10
1	G	110/118 (93%)	96 (87%)	14 (13%)	6	12
1	H	110/118 (93%)	97 (88%)	13 (12%)	8	14
2	I	87/92 (95%)	80 (92%)	7 (8%)	17	33
2	J	89/92 (97%)	81 (91%)	8 (9%)	14	26
2	K	85/92 (92%)	78 (92%)	7 (8%)	17	31
2	L	3/92 (3%)	3 (100%)	0	100	100
2	M	83/92 (90%)	77 (93%)	6 (7%)	21	39
2	N	83/92 (90%)	76 (92%)	7 (8%)	16	29
2	O	83/92 (90%)	76 (92%)	7 (8%)	16	29
2	P	88/92 (96%)	81 (92%)	7 (8%)	17	33
All	All	1476/1680 (88%)	1317 (89%)	159 (11%)	9	17

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	23	ARG
1	G	68	ILE

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Mol	Chain	Res	Type
2	O	145	LEU
1	F	58	GLU
1	F	117	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	72	GLN
1	G	27	ASN
2	N	215	HIS
1	E	76	GLN
1	F	61	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	500	-	9,9,9	1.40	1 (11%)	12,12,12	1.30	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SRT	A	600	-	9,9,9	1.38	1 (11%)	12,12,12	1.26	1 (8%)
3	SRT	B	500	-	9,9,9	1.34	1 (11%)	12,12,12	1.14	1 (8%)
3	SRT	B	600	-	9,9,9	1.30	1 (11%)	12,12,12	1.14	1 (8%)
3	SRT	C	500	-	9,9,9	1.25	1 (11%)	12,12,12	1.24	1 (8%)
3	SRT	C	600	-	9,9,9	1.18	0	12,12,12	1.12	1 (8%)
3	SRT	D	500	-	9,9,9	1.39	1 (11%)	12,12,12	1.37	2 (16%)
3	SRT	D	600	-	9,9,9	1.26	1 (11%)	12,12,12	1.19	1 (8%)
3	SRT	E	500	-	9,9,9	1.44	1 (11%)	12,12,12	1.24	2 (16%)
3	SRT	E	600	-	9,9,9	1.38	2 (22%)	12,12,12	1.15	1 (8%)
3	SRT	F	500	-	9,9,9	1.32	1 (11%)	12,12,12	1.23	1 (8%)
3	SRT	F	600	-	9,9,9	1.28	1 (11%)	12,12,12	1.15	1 (8%)
3	SRT	G	500	-	9,9,9	1.44	1 (11%)	12,12,12	1.36	3 (25%)
3	SRT	G	600	-	9,9,9	1.38	1 (11%)	12,12,12	1.02	0
3	SRT	H	500	-	9,9,9	1.36	2 (22%)	12,12,12	1.28	1 (8%)
3	SRT	H	600	-	9,9,9	1.24	1 (11%)	12,12,12	1.21	1 (8%)

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	A	500	-	-	0/12/12/12	0/0/0/0
3	SRT	A	600	-	-	0/12/12/12	0/0/0/0
3	SRT	B	500	-	-	0/12/12/12	0/0/0/0
3	SRT	B	600	-	-	0/12/12/12	0/0/0/0
3	SRT	C	500	-	-	0/12/12/12	0/0/0/0
3	SRT	C	600	-	-	0/12/12/12	0/0/0/0
3	SRT	D	500	-	-	0/12/12/12	0/0/0/0
3	SRT	D	600	-	-	0/12/12/12	0/0/0/0
3	SRT	E	500	-	-	0/12/12/12	0/0/0/0
3	SRT	E	600	-	-	0/12/12/12	0/0/0/0
3	SRT	F	500	-	-	0/12/12/12	0/0/0/0
3	SRT	F	600	-	-	0/12/12/12	0/0/0/0
3	SRT	G	500	-	-	0/12/12/12	0/0/0/0
3	SRT	G	600	-	-	0/12/12/12	0/0/0/0
3	SRT	H	500	-	-	0/12/12/12	0/0/0/0
3	SRT	H	600	-	-	0/12/12/12	0/0/0/0

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	SRT	C2-C1	-2.97	1.48	1.52
3	G	500	SRT	C3-C4	-2.78	1.49	1.52
3	D	500	SRT	C3-C4	-2.77	1.49	1.52
3	E	500	SRT	C3-C4	-2.74	1.49	1.52
3	A	500	SRT	C3-C4	-2.48	1.49	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	SRT	O3-C3-C2	-2.70	104.66	110.19
3	D	500	SRT	C2-C3-C4	-2.65	102.95	109.91
3	H	600	SRT	O3-C3-C2	-2.50	105.07	110.19
3	A	500	SRT	O2-C2-C3	-2.47	105.12	110.19
3	A	500	SRT	C2-C3-C4	-2.46	103.45	109.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.79	12 (8%) 11 8	29, 48, 131, 407	0
1	B	139/149 (93%)	0.92	16 (11%) 5 4	29, 47, 134, 410	0
1	C	139/149 (93%)	0.51	5 (3%) 41 37	31, 49, 120, 404	0
1	D	141/149 (94%)	0.59	10 (7%) 16 12	30, 49, 106, 403	0
1	E	139/149 (93%)	0.65	15 (10%) 6 5	31, 49, 121, 406	0
1	F	133/149 (89%)	0.39	6 (4%) 32 28	32, 49, 84, 139	0
1	G	139/149 (93%)	0.46	6 (4%) 34 30	31, 48, 119, 406	0
1	H	139/149 (93%)	0.57	10 (7%) 15 12	32, 51, 115, 408	0
2	I	94/98 (95%)	0.40	5 (5%) 25 22	31, 48, 96, 129	0
2	J	95/98 (96%)	0.54	5 (5%) 25 22	31, 46, 98, 129	0
2	K	92/98 (93%)	0.60	8 (8%) 10 8	33, 49, 101, 131	0
2	L	4/98 (4%)	1.28	0 100 100	40, 47, 59, 82	0
2	M	90/98 (91%)	0.68	6 (6%) 17 15	36, 51, 85, 109	0
2	N	89/98 (90%)	0.40	3 (3%) 43 39	31, 47, 79, 104	0
2	O	89/98 (90%)	0.70	9 (10%) 7 5	31, 51, 86, 129	0
2	P	94/98 (95%)	0.51	6 (6%) 19 16	34, 48, 99, 140	0
All	All	1756/1976 (88%)	0.59	122 (6%) 17 14	29, 49, 103, 410	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	18.2
1	B	73	GLU	14.0
1	E	75	SER	10.3
1	D	72	GLN	10.2
1	B	75	SER	9.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SRT	G	500	10/10	0.34	4.19	69,82,99,109	0
3	SRT	C	500	10/10	0.28	3.65	71,83,100,112	0
3	SRT	H	600	10/10	0.29	2.63	44,67,85,86	0
3	SRT	A	500	10/10	0.29	2.01	59,83,92,105	0
3	SRT	G	600	10/10	0.22	1.72	44,61,75,85	0
3	SRT	D	600	10/10	0.20	1.35	53,68,75,81	0
3	SRT	E	500	10/10	0.24	1.21	74,83,96,108	0
3	SRT	C	600	10/10	0.19	1.06	37,62,75,78	0
3	SRT	D	500	10/10	0.23	0.80	75,84,102,108	0
3	SRT	F	500	10/10	0.24	0.77	73,81,97,110	0
3	SRT	A	600	10/10	0.21	0.63	49,60,76,77	0
3	SRT	H	500	10/10	0.22	0.54	73,83,99,104	0
3	SRT	E	600	10/10	0.18	0.32	48,63,74,81	0
3	SRT	F	600	10/10	0.19	0.17	42,66,81,84	0
3	SRT	B	500	10/10	0.17	0.05	58,76,96,104	0
3	SRT	B	600	10/10	0.17	-0.06	41,64,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.