WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 06:27 am GMT

PDB ID	:	6HCS
Title	:	Crystal structure of CaM-peptide complex containing AzF at position 108
Authors	:	Creon, A.; Josts, I.; Tidow, H.
Deposited on	:	2018-08-16
Resolution	:	2.00 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*
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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
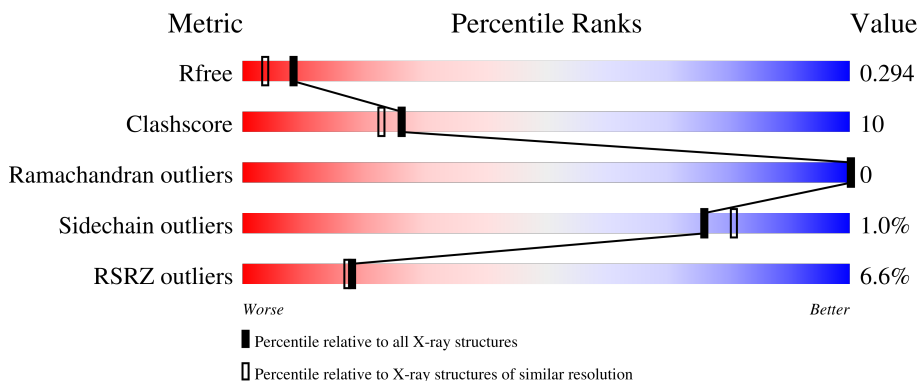
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	167	% / 73% / 8% • 18%
1	C	167	2% / 69% / 13% • 17%
1	E	167	9% / 59% / 23% • 17%
1	G	167	9% / 60% / 22% • 17%
2	B	25	72% • 24%

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Mol	Chain	Length	Quality of chain
2	D	25	8% ▮▮ 76% · · 16%
2	F	25	12% ▮▮ 36% 32% · 28%
2	H	25	4% ▮ 44% 28% 28%

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
1	4II	E	108	-	-	X	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5239 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1089	670	178	233	8			
1	C	139	Total	C	N	O	S	0	0	0
			1106	680	180	237	9			
1	E	138	Total	C	N	O	S	0	0	0
			1094	673	179	234	8			
1	G	138	Total	C	N	O	S	0	0	0
			1094	673	179	234	8			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	4II	VAL	engineered mutation	UNP P0DP23
A	149	LEU	-	expression tag	UNP P0DP23
A	150	GLU	-	expression tag	UNP P0DP23
A	151	GLY	-	expression tag	UNP P0DP23
A	152	THR	-	expression tag	UNP P0DP23
A	153	GLY	-	expression tag	UNP P0DP23
A	154	LEU	-	expression tag	UNP P0DP23
A	155	GLU	-	expression tag	UNP P0DP23
A	156	VAL	-	expression tag	UNP P0DP23
A	157	LEU	-	expression tag	UNP P0DP23
A	158	PHE	-	expression tag	UNP P0DP23
A	159	GLN	-	expression tag	UNP P0DP23
A	160	GLY	-	expression tag	UNP P0DP23
A	161	HIS	-	expression tag	UNP P0DP23
A	162	HIS	-	expression tag	UNP P0DP23
A	163	HIS	-	expression tag	UNP P0DP23
A	164	HIS	-	expression tag	UNP P0DP23
A	165	HIS	-	expression tag	UNP P0DP23
A	166	HIS	-	expression tag	UNP P0DP23
C	108	4II	VAL	engineered mutation	UNP P0DP23
C	149	LEU	-	expression tag	UNP P0DP23

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Chain	Residue	Modelled	Actual	Comment	Reference
C	150	GLU	-	expression tag	UNP P0DP23
C	151	GLY	-	expression tag	UNP P0DP23
C	152	THR	-	expression tag	UNP P0DP23
C	153	GLY	-	expression tag	UNP P0DP23
C	154	LEU	-	expression tag	UNP P0DP23
C	155	GLU	-	expression tag	UNP P0DP23
C	156	VAL	-	expression tag	UNP P0DP23
C	157	LEU	-	expression tag	UNP P0DP23
C	158	PHE	-	expression tag	UNP P0DP23
C	159	GLN	-	expression tag	UNP P0DP23
C	160	GLY	-	expression tag	UNP P0DP23
C	161	HIS	-	expression tag	UNP P0DP23
C	162	HIS	-	expression tag	UNP P0DP23
C	163	HIS	-	expression tag	UNP P0DP23
C	164	HIS	-	expression tag	UNP P0DP23
C	165	HIS	-	expression tag	UNP P0DP23
C	166	HIS	-	expression tag	UNP P0DP23
E	108	4II	VAL	engineered mutation	UNP P0DP23
E	149	LEU	-	expression tag	UNP P0DP23
E	150	GLU	-	expression tag	UNP P0DP23
E	151	GLY	-	expression tag	UNP P0DP23
E	152	THR	-	expression tag	UNP P0DP23
E	153	GLY	-	expression tag	UNP P0DP23
E	154	LEU	-	expression tag	UNP P0DP23
E	155	GLU	-	expression tag	UNP P0DP23
E	156	VAL	-	expression tag	UNP P0DP23
E	157	LEU	-	expression tag	UNP P0DP23
E	158	PHE	-	expression tag	UNP P0DP23
E	159	GLN	-	expression tag	UNP P0DP23
E	160	GLY	-	expression tag	UNP P0DP23
E	161	HIS	-	expression tag	UNP P0DP23
E	162	HIS	-	expression tag	UNP P0DP23
E	163	HIS	-	expression tag	UNP P0DP23
E	164	HIS	-	expression tag	UNP P0DP23
E	165	HIS	-	expression tag	UNP P0DP23
E	166	HIS	-	expression tag	UNP P0DP23
G	108	4II	VAL	engineered mutation	UNP P0DP23
G	149	LEU	-	expression tag	UNP P0DP23
G	150	GLU	-	expression tag	UNP P0DP23
G	151	GLY	-	expression tag	UNP P0DP23
G	152	THR	-	expression tag	UNP P0DP23
G	153	GLY	-	expression tag	UNP P0DP23

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Chain	Residue	Modelled	Actual	Comment	Reference
G	154	LEU	-	expression tag	UNP P0DP23
G	155	GLU	-	expression tag	UNP P0DP23
G	156	VAL	-	expression tag	UNP P0DP23
G	157	LEU	-	expression tag	UNP P0DP23
G	158	PHE	-	expression tag	UNP P0DP23
G	159	GLN	-	expression tag	UNP P0DP23
G	160	GLY	-	expression tag	UNP P0DP23
G	161	HIS	-	expression tag	UNP P0DP23
G	162	HIS	-	expression tag	UNP P0DP23
G	163	HIS	-	expression tag	UNP P0DP23
G	164	HIS	-	expression tag	UNP P0DP23
G	165	HIS	-	expression tag	UNP P0DP23
G	166	HIS	-	expression tag	UNP P0DP23

- Molecule 2 is a protein called Calcium/calmodulin-dependent protein kinase type II subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	19	Total	C	N	O	S	0	0	0
			150	95	31	23	1			
2	D	21	Total	C	N	O	S	0	0	0
			169	108	34	26	1			
2	F	18	Total	C	N	O	S	0	0	0
			139	89	27	22	1			
2	H	18	Total	C	N	O	S	0	0	0
			139	89	27	22	1			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	C	4	Total	Ca	0	0
			4	4		
3	E	4	Total	Ca	0	0
			4	4		
3	G	4	Total	Ca	0	0
			4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total 100	O 100	0	0
4	B	5	Total 5	O 5	0	0
4	C	94	Total 94	O 94	0	0
4	D	6	Total 6	O 6	0	0
4	E	18	Total 18	O 18	0	0
4	F	2	Total 2	O 2	0	0
4	G	17	Total 17	O 17	0	0
4	H	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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.
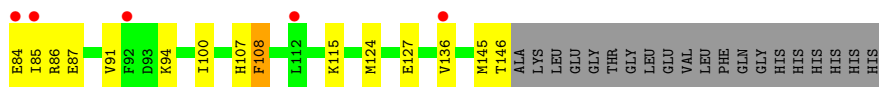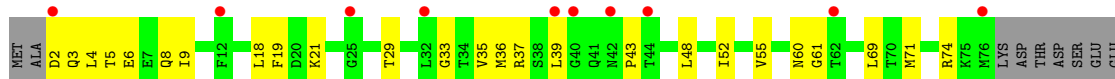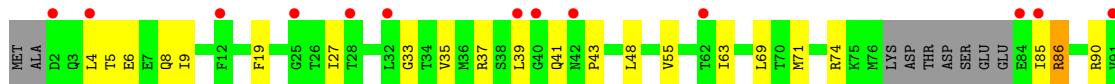
- Molecule 1: Calmodulin-1
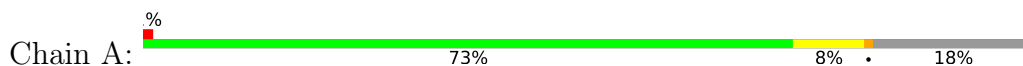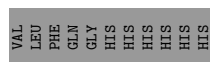
Chain A:

- Molecule 1: Calmodulin-1

Chain C:

- Molecule 1: Calmodulin-1

Chain E:

- Molecule 1: Calmodulin-1

Chain G:

• Molecule 2: Calcium/calmodulin-dependent protein kinase type II subunit beta

Chain B:

72%   •   24%
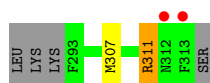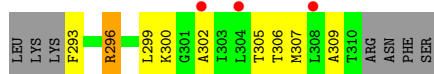

• Molecule 2: Calcium/calmodulin-dependent protein kinase type II subunit beta

8%

Chain D:

76%   • •   16%

• Molecule 2: Calcium/calmodulin-dependent protein kinase type II subunit beta

12%

Chain F:

36%   32%   •   28%

• Molecule 2: Calcium/calmodulin-dependent protein kinase type II subunit beta

4%

Chain H:

44%   28%   28%

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.26Å 37.21Å 121.19Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	43.12 – 2.00 43.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.12-2.00) 97.9 (43.12-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.37 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.260 , 0.294 0.262 , 0.294	Depositor DCC
R_{free} test set	2267 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.8	EDS
L-test for twinning [2]	$<\|L\|> = 0.46$, $<L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5239	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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 88.09 % 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 5.5273e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<\|L\|>$, $<L^2>$ 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: 4II, CA

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	0.47	0/1085	0.57	0/1454
1	C	0.47	0/1102	0.59	0/1476
1	E	0.32	0/1090	0.50	0/1461
1	G	0.36	0/1090	0.51	0/1461
2	B	0.39	0/150	0.57	0/198
2	D	0.42	0/170	0.61	0/225
2	F	0.43	0/139	0.56	0/184
2	H	0.33	0/139	0.46	0/184
All	All	0.41	0/4965	0.54	0/6643

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	0	1
1	C	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	HIS	Mainchain
1	C	107	HIS	Mainchain

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Mol	Chain	Res	Type	Group
1	E	107	HIS	Mainchain

5.2 Too-close contacts (i)

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	1089	0	1006	12	0
1	C	1106	0	1021	14	0
1	E	1094	0	1008	37	0
1	G	1094	0	1008	28	0
2	B	150	0	171	1	0
2	D	169	0	186	4	0
2	F	139	0	158	15	0
2	H	139	0	157	10	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
3	E	4	0	0	0	0
3	G	4	0	0	0	0
4	A	100	0	0	1	0
4	B	5	0	0	0	0
4	C	94	0	0	2	0
4	D	6	0	0	1	0
4	E	18	0	0	1	0
4	F	2	0	0	1	0
4	G	17	0	0	2	0
4	H	1	0	0	1	0
All	All	5239	0	4715	101	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 10.

All (101) 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:E:108:4II:CZ	1:E:108:4II:N1	1.68	1.49
1:E:145:MET:HA	2:F:300:LYS:HE2	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ARG:HG3	1:E:87:GLU:HG3	1.57	0.85
2:F:293:PHE:N	4:F:401:HOH:O	2.16	0.77
1:E:5:THR:HG23	1:E:8:GLN:H	1.51	0.76
1:A:106:ARG:NH1	1:A:118:ASP:OD1	2.21	0.71
1:E:4:LEU:HD21	1:E:69:LEU:HD11	1.73	0.71
1:G:5:THR:HG23	1:G:8:GLN:H	1.56	0.70
1:G:110:THR:HG23	1:G:115:LYS:HE2	1.74	0.70
1:A:106:ARG:NH2	1:A:116:LEU:O	2.25	0.69
1:C:106:ARG:NH2	1:C:116:LEU:O	2.25	0.69
1:E:108:4II:N3	2:F:305:THR:OG1	2.27	0.68
1:E:108:4II:CZ	1:E:108:4II:N2	2.49	0.67
1:E:29:THR:HG22	1:E:52:ILE:HG13	1.76	0.67
1:C:146:THR:O	4:C:301:HOH:O	2.13	0.66
1:G:4:LEU:HD21	1:G:69:LEU:HD11	1.77	0.66
1:G:74:ARG:NH2	4:G:301:HOH:O	2.27	0.66
1:E:39:LEU:HD21	2:F:306:THR:HG23	1.77	0.66
1:A:108:4II:N3	1:A:112:LEU:HD11	2.11	0.66
2:F:307:MET:HA	2:F:307:MET:HE2	1.77	0.64
2:D:311:ARG:NH1	4:D:401:HOH:O	2.31	0.64
1:E:18:LEU:HD13	1:E:108:4II:N3	2.13	0.64
1:E:127:GLU:OE1	2:F:296:ARG:NH2	2.32	0.62
1:E:108:4II:N2	2:F:305:THR:HB	2.15	0.62
1:E:36:MET:HE2	1:E:43:PRO:HG3	1.82	0.62
1:E:145:MET:HG2	2:F:300:LYS:HZ1	1.63	0.62
1:C:48:LEU:HA	1:C:51:MET:HE3	1.83	0.60
2:D:311:ARG:O	2:D:311:ARG:HG3	2.02	0.59
1:C:106:ARG:NH1	1:C:118:ASP:OD2	2.29	0.59
1:E:108:4II:N3	2:F:305:THR:CB	2.66	0.58
1:G:108:4II:N3	2:H:305:THR:HB	2.17	0.58
2:H:293:PHE:N	4:H:401:HOH:O	2.36	0.57
1:A:84:GLU:HG3	1:A:87:GLU:H	1.70	0.57
1:G:122:ASP:O	1:G:126:ARG:HG2	2.06	0.56
1:G:101:SER:HA	1:G:135:GLN:HG2	1.87	0.55
1:E:71:MET:HA	1:E:74:ARG:HE	1.70	0.55
1:G:19:PHE:CD2	1:G:35:VAL:HG11	2.42	0.55
1:E:146:THR:O	4:E:301:HOH:O	2.18	0.55
1:G:39:LEU:HB3	1:G:41:GLN:OE1	2.08	0.54
1:G:37:ARG:HD3	1:G:43:PRO:HD2	1.89	0.54
1:G:35:VAL:HG23	1:G:112:LEU:HD21	1.90	0.54
1:E:85:ILE:HD13	1:E:145:MET:SD	2.47	0.54
1:A:29:THR:HG22	1:A:52:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:MET:HE2	2:F:299:LEU:HB2	1.91	0.53
1:E:55:VAL:HG22	1:E:71:MET:HG3	1.91	0.53
1:G:121:VAL:HA	1:G:124:MET:HE3	1.91	0.52
1:E:145:MET:CG	2:F:300:LYS:HZ1	2.23	0.51
1:C:56:ASP:HB2	4:C:327:HOH:O	2.11	0.51
1:C:84:GLU:HG2	2:D:311:ARG:HD3	1.93	0.50
1:E:21:LYS:HE3	1:E:35:VAL:HG12	1.92	0.50
1:E:43:PRO:HG2	1:E:48:LEU:HD21	1.92	0.50
1:E:108:4II:N3	2:F:302:ALA:HA	2.27	0.50
1:C:74:ARG:HG2	1:C:75:LYS:N	2.27	0.49
1:G:6:GLU:HA	1:G:9:ILE:HD12	1.95	0.49
1:C:85:ILE:CD1	1:C:142:VAL:HA	2.44	0.48
1:A:48:LEU:HA	1:A:51:MET:HE3	1.94	0.48
1:C:108:4II:N3	1:C:112:LEU:HD11	2.28	0.48
2:D:307:MET:O	2:D:311:ARG:HG2	2.14	0.48
1:E:84:GLU:O	1:E:86:ARG:HG2	2.14	0.48
1:C:85:ILE:HD13	1:C:142:VAL:HA	1.95	0.47
1:E:145:MET:HG2	2:F:300:LYS:NZ	2.29	0.47
1:G:39:LEU:HD23	2:H:309:ALA:HB3	1.96	0.47
2:H:300:LYS:HZ1	2:H:304:LEU:HG	1.79	0.47
1:G:139:GLU:HA	1:G:142:VAL:HG22	1.96	0.47
1:E:6:GLU:HA	1:E:9:ILE:HD12	1.96	0.47
2:H:300:LYS:HZ3	2:H:303:ILE:HB	1.79	0.47
1:E:37:ARG:HD3	1:E:43:PRO:HD2	1.95	0.47
1:E:39:LEU:HG	1:E:91:VAL:HG11	1.97	0.47
1:G:39:LEU:HD12	1:G:39:LEU:HA	1.73	0.46
1:A:108:4II:N2	1:A:112:LEU:HD11	2.30	0.46
1:C:29:THR:HG22	1:C:52:ILE:HG13	1.98	0.46
1:G:5:THR:HG22	1:G:8:GLN:OE1	2.15	0.46
2:H:300:LYS:NZ	2:H:304:LEU:HG	2.31	0.46
1:C:91:VAL:O	1:C:94:LYS:HE3	2.15	0.45
1:G:55:VAL:HG22	1:G:71:MET:HG3	1.99	0.45
1:G:119:GLU:O	1:G:123:GLU:HG3	2.17	0.45
1:A:108:4II:N3	2:B:305:THR:HB	2.32	0.45
1:C:55:VAL:HB	1:C:63:ILE:HD12	1.99	0.45
1:G:33:GLY:O	1:G:37:ARG:HG2	2.16	0.44
1:E:2:ASP:OD1	1:E:3:GLN:N	2.50	0.44
1:E:19:PHE:CD1	1:E:35:VAL:HG21	2.52	0.44
1:G:126:ARG:HG2	1:G:126:ARG:H	1.64	0.44
1:G:145:MET:HA	2:H:300:LYS:HE2	2.00	0.44
1:E:19:PHE:CE1	1:E:35:VAL:HG21	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HD13	1:A:142:VAL:HA	2.00	0.43
1:A:85:ILE:CD1	1:A:142:VAL:HA	2.49	0.43
1:E:33:GLY:O	1:E:37:ARG:HG2	2.19	0.43
1:G:143:GLN:NE2	4:G:305:HOH:O	2.50	0.43
1:E:100:ILE:HB	1:E:136:VAL:HB	2.00	0.43
1:E:108:4II:N2	2:F:305:THR:CB	2.80	0.42
1:A:30:LYS:HG3	4:A:332:HOH:O	2.18	0.42
1:C:21:LYS:HE2	1:C:34:THR:HG21	2.00	0.42
1:G:86:ARG:O	1:G:90:ARG:HG3	2.19	0.42
1:G:19:PHE:CE1	2:H:305:THR:HG23	2.55	0.42
1:G:85:ILE:HA	2:H:307:MET:SD	2.59	0.42
2:H:300:LYS:NZ	2:H:303:ILE:HB	2.36	0.41
1:E:39:LEU:HD22	2:F:309:ALA:CB	2.51	0.41
1:E:60:ASN:OD1	1:E:61:GLY:N	2.53	0.41
1:A:84:GLU:OE1	1:A:84:GLU:HA	2.21	0.40
1:G:43:PRO:HG2	1:G:48:LEU:HD21	2.02	0.40
1:G:27:ILE:HB	1:G:63:ILE:HB	2.03	0.40

There are no symmetry-related clashes.

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	132/167 (79%)	132 (100%)	0	0	100	100
1	C	134/167 (80%)	133 (99%)	1 (1%)	0	100	100
1	E	133/167 (80%)	129 (97%)	4 (3%)	0	100	100
1	G	133/167 (80%)	128 (96%)	5 (4%)	0	100	100
2	B	17/25 (68%)	17 (100%)	0	0	100	100
2	D	19/25 (76%)	17 (90%)	2 (10%)	0	100	100
2	F	16/25 (64%)	16 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	16/25 (64%)	16 (100%)	0	0	100	100
All	All	600/768 (78%)	588 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	116/141 (82%)	116 (100%)	0	100	100
1	C	118/141 (84%)	118 (100%)	0	100	100
1	E	116/141 (82%)	114 (98%)	2 (2%)	60	65
1	G	116/141 (82%)	115 (99%)	1 (1%)	78	83
2	B	15/21 (71%)	15 (100%)	0	100	100
2	D	17/21 (81%)	16 (94%)	1 (6%)	19	15
2	F	14/21 (67%)	13 (93%)	1 (7%)	14	10
2	H	14/21 (67%)	14 (100%)	0	100	100
All	All	526/648 (81%)	521 (99%)	5 (1%)	76	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	311	ARG
1	E	94	LYS
1	E	115	LYS
2	F	296	ARG
1	G	86	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	4II	G	108	2,1	12,14,15	4.20	9 (75%)	13,17,19	1.48	3 (23%)
1	4II	C	108	1	12,14,15	4.28	9 (75%)	13,17,19	1.86	3 (23%)
1	4II	E	108	1	12,14,15	4.23	9 (75%)	13,17,19	0.93	0
1	4II	A	108	1	12,14,15	4.29	8 (66%)	13,17,19	1.86	4 (30%)

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
1	4II	G	108	2,1	-	1/8/9/11	0/1/1/1
1	4II	C	108	1	-	0/8/9/11	0/1/1/1
1	4II	E	108	1	-	1/8/9/11	0/1/1/1
1	4II	A	108	1	-	0/8/9/11	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	108	4II	CZ-N1	9.93	1.68	1.43
1	A	108	4II	CZ-N1	9.67	1.67	1.43
1	C	108	4II	CZ-N1	9.55	1.67	1.43
1	G	108	4II	CZ-N1	9.54	1.67	1.43
1	A	108	4II	CB-CA	5.55	1.65	1.53
1	G	108	4II	CD2-CG	-5.53	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	4II	CD2-CG	-5.46	1.27	1.38
1	C	108	4II	CB-CA	5.33	1.65	1.53
1	E	108	4II	CD2-CG	-5.15	1.27	1.38
1	C	108	4II	CD2-CG	-5.13	1.27	1.38
1	E	108	4II	CB-CG	5.05	1.63	1.51
1	C	108	4II	CB-CG	4.78	1.62	1.51
1	E	108	4II	CB-CA	4.76	1.64	1.53
1	A	108	4II	CB-CG	4.51	1.62	1.51
1	G	108	4II	CB-CG	4.47	1.62	1.51
1	G	108	4II	CB-CA	4.29	1.62	1.53
1	C	108	4II	CE1-CZ	-3.86	1.31	1.39
1	G	108	4II	CE1-CZ	-3.78	1.31	1.39
1	C	108	4II	O-C	3.49	1.33	1.19
1	E	108	4II	CE1-CZ	-3.40	1.32	1.39
1	A	108	4II	O-C	3.34	1.33	1.19
1	A	108	4II	CE1-CZ	-3.30	1.32	1.39
1	E	108	4II	O-C	3.28	1.33	1.19
1	G	108	4II	O-C	3.24	1.32	1.19
1	A	108	4II	CE2-CZ	-2.88	1.33	1.39
1	G	108	4II	CD1-CG	-2.71	1.33	1.38
1	G	108	4II	CA-N	-2.66	1.40	1.48
1	C	108	4II	CE2-CZ	-2.61	1.34	1.39
1	A	108	4II	CA-N	-2.49	1.40	1.48
1	E	108	4II	CE2-CZ	-2.49	1.34	1.39
1	G	108	4II	CE2-CZ	-2.47	1.34	1.39
1	C	108	4II	CD1-CG	-2.41	1.33	1.38
1	C	108	4II	CA-N	-2.28	1.41	1.48
1	E	108	4II	CA-N	-2.12	1.41	1.48
1	E	108	4II	CD1-CG	-2.01	1.34	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	4II	CG-CB-CA	-4.78	104.43	114.10
1	A	108	4II	CG-CB-CA	-4.22	105.55	114.10
1	G	108	4II	CG-CB-CA	2.74	119.65	114.10
1	G	108	4II	CD1-CG-CD2	2.61	122.27	118.17
1	A	108	4II	CD1-CG-CD2	2.60	122.26	118.17
1	C	108	4II	CD1-CG-CD2	2.39	121.93	118.17
1	C	108	4II	CZ-N1-N2	2.34	120.66	116.02
1	A	108	4II	CB-CG-CD2	-2.20	116.53	120.91
1	A	108	4II	CZ-N1-N2	2.11	120.22	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	108	4II	CZ-N1-N2	2.10	120.19	116.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	108	4II	CZ-N1-N2-N3
1	E	108	4II	CZ-N1-N2-N3

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	108	4II	1	0
1	C	108	4II	1	0
1	E	108	4II	8	0
1	A	108	4II	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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(Å²)	Q<0.9
1	A	136/167 (81%)	-0.06	1 (0%)	87	87	20, 32, 47, 75	0
1	C	138/167 (82%)	0.11	4 (2%)	51	50	18, 35, 53, 77	0
1	E	137/167 (82%)	0.78	15 (10%)	5	5	46, 72, 97, 111	0
1	G	137/167 (82%)	0.70	15 (10%)	5	5	39, 59, 83, 91	0
2	B	19/25 (76%)	-0.32	0	100	100	23, 28, 37, 54	0
2	D	21/25 (84%)	0.29	2 (9%)	8	7	23, 28, 58, 78	0
2	F	18/25 (72%)	1.11	3 (16%)	1	1	52, 61, 78, 88	0
2	H	18/25 (72%)	0.81	1 (5%)	24	23	48, 55, 65, 69	0
All	All	624/768 (81%)	0.39	41 (6%)	18	17	18, 48, 84, 111	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	ASP	6.6
1	E	2	ASP	5.2
1	G	39	LEU	4.7
2	D	312	ASN	4.4
2	F	308	LEU	4.2
1	C	75	LYS	4.1
2	H	308	LEU	3.9
1	G	84	GLU	3.6
1	E	92	PHE	3.6
2	D	313	PHE	3.5
1	E	39	LEU	3.3
1	E	112	LEU	3.1
1	E	62	THR	3.0
1	E	12	PHE	2.9
1	G	42	ASN	2.8
1	E	76	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	32	LEU	2.7
2	F	304	LEU	2.6
1	G	62	THR	2.5
1	E	84	GLU	2.5
1	E	32	LEU	2.5
1	C	76	MET	2.5
1	G	4	LEU	2.4
1	E	40	GLY	2.4
2	F	302	ALA	2.4
1	G	12	PHE	2.3
1	G	112	LEU	2.3
1	A	75	LYS	2.3
1	G	85	ILE	2.3
1	E	25	GLY	2.3
1	E	85	ILE	2.2
1	G	25	GLY	2.2
1	E	136	VAL	2.2
1	E	42	ASN	2.2
1	G	92	PHE	2.1
1	G	28	THR	2.1
1	C	3	GLN	2.1
1	C	2	ASP	2.1
1	G	91	VAL	2.1
1	G	40	GLY	2.0
1	E	44	THR	2.0

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

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(Å^2)	Q<0.9
1	4II	G	108	14/15	0.54	0.34	74,79,82,83	0
1	4II	E	108	14/15	0.65	0.40	74,79,83,84	0
1	4II	A	108	14/15	0.90	0.17	23,29,53,53	0
1	4II	C	108	14/15	0.91	0.16	19,29,52,55	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å^2)	Q<0.9
3	CA	E	204	1/1	0.76	0.07	73,73,73,73	0
3	CA	E	203	1/1	0.90	0.07	61,61,61,61	0
3	CA	E	201	1/1	0.91	0.08	74,74,74,74	0
3	CA	G	204	1/1	0.92	0.04	74,74,74,74	0
3	CA	G	201	1/1	0.94	0.06	60,60,60,60	0
3	CA	A	204	1/1	0.95	0.18	29,29,29,29	0
3	CA	G	202	1/1	0.95	0.05	72,72,72,72	0
3	CA	E	202	1/1	0.95	0.09	87,87,87,87	0
3	CA	C	201	1/1	0.97	0.11	37,37,37,37	0
3	CA	C	202	1/1	0.97	0.16	47,47,47,47	0
3	CA	G	203	1/1	0.97	0.04	58,58,58,58	0
3	CA	A	202	1/1	0.97	0.10	33,33,33,33	0
3	CA	C	203	1/1	0.99	0.08	17,17,17,17	0
3	CA	A	203	1/1	0.99	0.13	25,25,25,25	0
3	CA	A	201	1/1	0.99	0.04	24,24,24,24	0
3	CA	C	204	1/1	1.00	0.11	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.