



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:23 PM GMT

PDB ID : 3X1L
Title : Crystal Structure of the CRISPR-Cas RNA Silencing Cmr Complex Bound to a Target Analog
Authors : Osawa, T.; Numata, T.
Deposited on : 2014-11-20
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

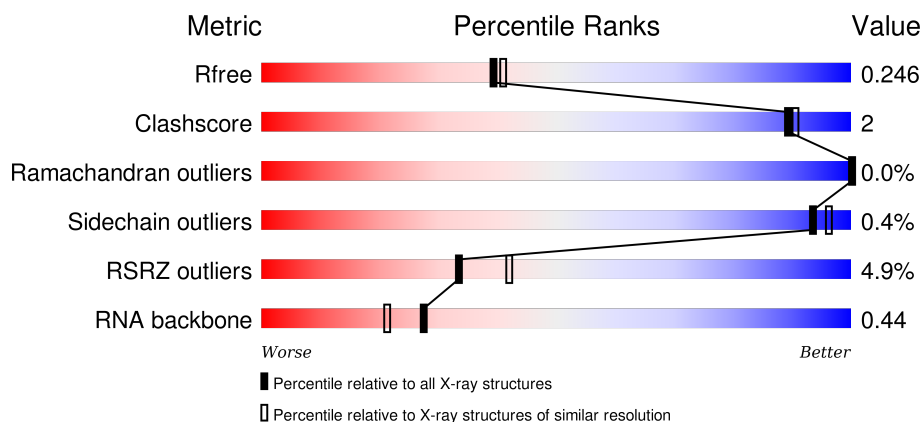
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)
RNA backbone	2183	1118 (2.80-1.40)

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. 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	677	<div> <div>4%</div> <div>79%</div> <div>6%</div> <div>15%</div> </div>
2	B	322	<div> <div>%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
3	C	357	<div> <div>%</div> <div>85%</div> <div>6%</div> <div>10%</div> </div>
3	D	357	<div> <div>4%</div> <div>85%</div> <div>7%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	357	<div><div></div><div>10%</div><div>85%</div><div>8%</div><div>8%</div></div>
4	F	155	<div><div></div><div>5%</div><div>89%</div><div>5%</div><div>6%</div></div>
4	G	155	<div><div></div><div>6%</div><div>88%</div><div>10%</div><div></div></div>
5	H	349	<div><div></div><div>7%</div><div>81%</div><div></div><div>15%</div></div>
6	I	39	<div><div></div><div>5%</div><div>56%</div><div>26%</div><div>18%</div></div>
7	J	31	<div><div></div><div></div><div>65%</div><div>6%</div><div>29%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19952 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 CRISPR system Cmr subunit Cmr2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	0	0
			4470	2920	749	789	12			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	MET	-	EXPRESSION TAG	UNP Q8U1S6
A	196	GLY	-	EXPRESSION TAG	UNP Q8U1S6
A	197	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	198	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	199	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	200	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	201	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	202	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	203	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	204	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	205	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	206	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	207	GLY	-	EXPRESSION TAG	UNP Q8U1S6
A	208	LEU	-	EXPRESSION TAG	UNP Q8U1S6
A	209	VAL	-	EXPRESSION TAG	UNP Q8U1S6
A	210	PRO	-	EXPRESSION TAG	UNP Q8U1S6
A	211	ARG	-	EXPRESSION TAG	UNP Q8U1S6
A	212	GLY	-	EXPRESSION TAG	UNP Q8U1S6
A	213	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	214	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	215	MET	-	EXPRESSION TAG	UNP Q8U1S6

- Molecule 2 is a protein called CRISPR system Cmr subunit Cmr3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2458	1611	394	449	4			

- Molecule 3 is a protein called Cmr4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	322	Total	C	N	O	S	0	0	0
			2405	1549	411	444	1			
3	D	331	Total	C	N	O	S	0	0	0
			2428	1571	413	442	2			
3	E	330	Total	C	N	O	S	0	0	0
			2395	1550	410	434	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	EXPRESSION TAG	UNP O28416
C	0	GLY	-	EXPRESSION TAG	UNP O28416
D	-1	MET	-	EXPRESSION TAG	UNP O28416
D	0	GLY	-	EXPRESSION TAG	UNP O28416
E	-1	MET	-	EXPRESSION TAG	UNP O28416
E	0	GLY	-	EXPRESSION TAG	UNP O28416

- Molecule 4 is a protein called CRISPR system Cmr subunit Cmr5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	146	Total	C	N	O	S	0	0	0
			1110	722	180	206	2			
4	G	152	Total	C	N	O	S	0	0	0
			1167	753	186	226	2			

- Molecule 5 is a protein called Cmr6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	297	Total	C	N	O	S	0	0	0
			2260	1469	363	425	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	344	HIS	-	EXPRESSION TAG	UNP O28418
H	345	HIS	-	EXPRESSION TAG	UNP O28418

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Chain	Residue	Modelled	Actual	Comment	Reference
H	346	HIS	-	EXPRESSION TAG	UNP O28418
H	347	HIS	-	EXPRESSION TAG	UNP O28418
H	348	HIS	-	EXPRESSION TAG	UNP O28418
H	349	HIS	-	EXPRESSION TAG	UNP O28418

- Molecule 6 is a RNA chain called RNA (32-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	32	Total	C	N	O	P	0	0	0
			679	304	117	227	31			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*GP*CP*TP*CP*TP*CP*AP*GP*CP*CP*GP*CP*AP*AP*GP*GP*AP*CP*CP*GP*CP*AP*TP*AP*CP*TP*AP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	22	Total	C	N	O	P	0	0	0
			448	212	88	126	22			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	32	Total	O	0	0
			32	32		
10	B	23	Total	O	0	0
			23	23		
10	C	16	Total	O	0	0
			16	16		
10	D	14	Total	O	0	0
			14	14		

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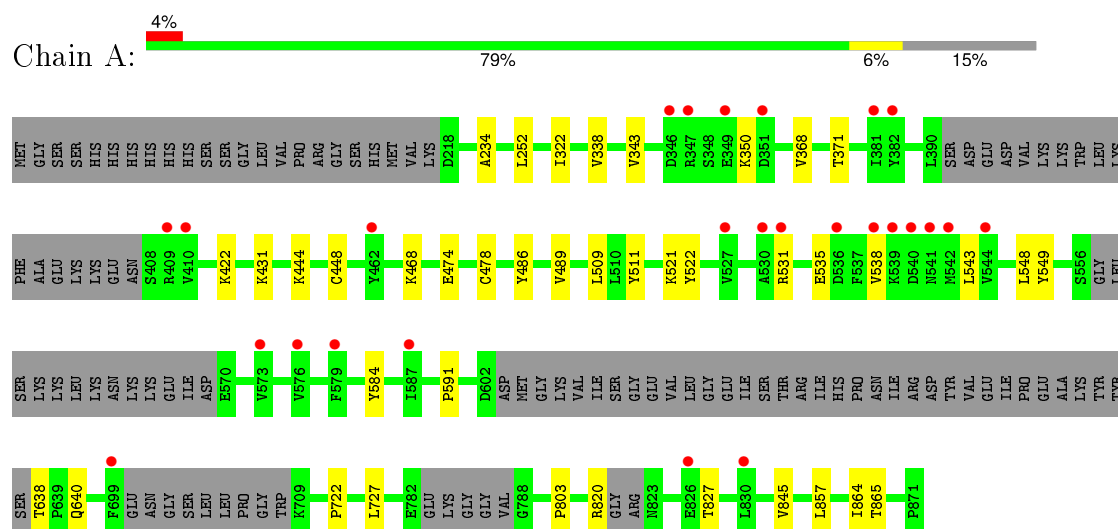
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	13	Total 13	O 13	0	0
10	G	5	Total 5	O 5	0	0
10	H	4	Total 4	O 4	0	0
10	I	23	Total 23	O 23	0	0

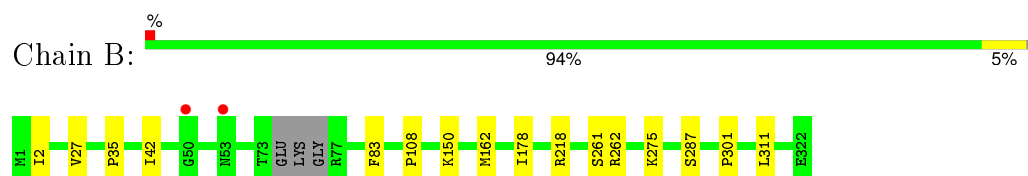
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

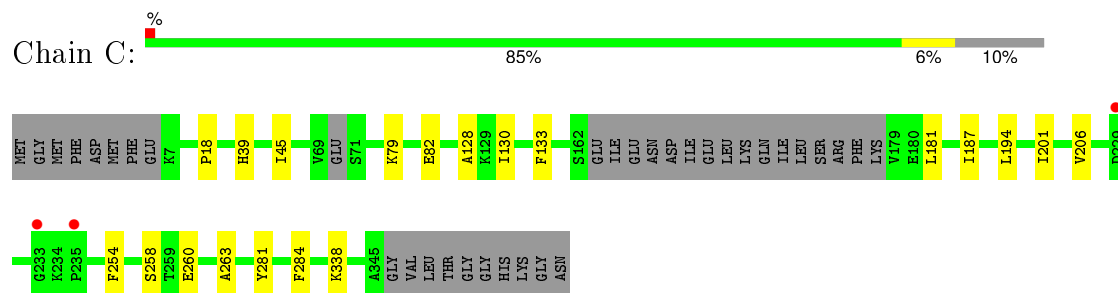
• Molecule 1: CRISPR system Cmr subunit Cmr2



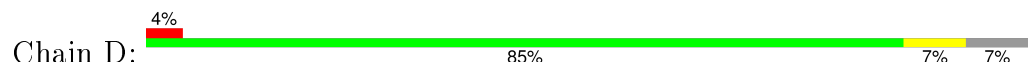
• Molecule 2: CRISPR system Cmr subunit Cmr3

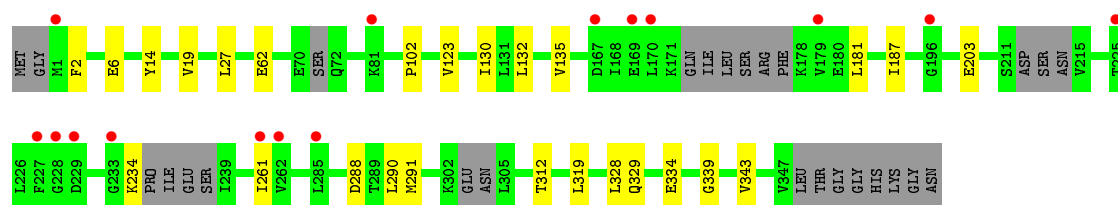


• Molecule 3: Cmr4

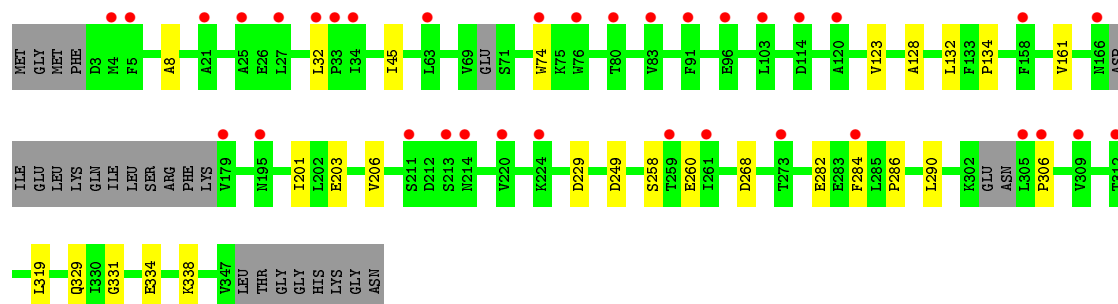
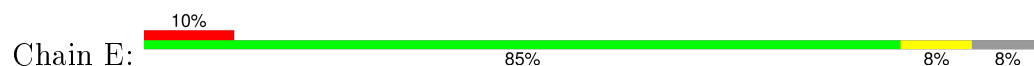


• Molecule 3: Cmr4

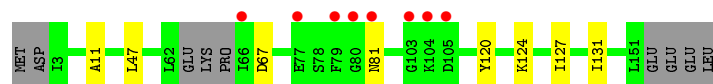
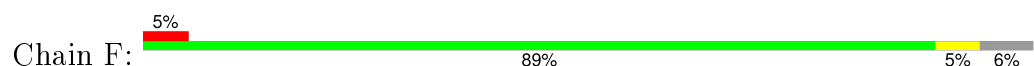




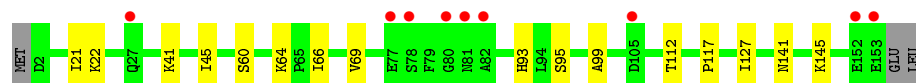
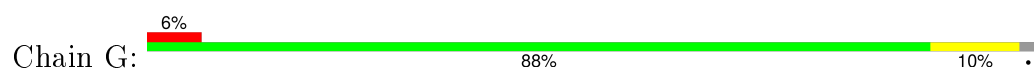
- Molecule 3: Cmr4



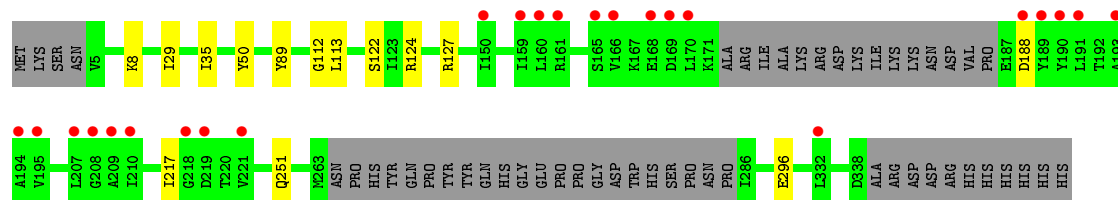
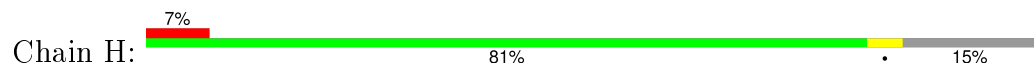
- Molecule 4: CRISPR system Cmr subunit Cmr5



- Molecule 4: CRISPR system Cmr subunit Cmr5

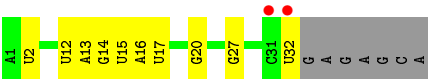


- Molecule 5: Cmr6

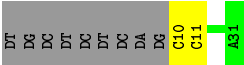


- Molecule 6: RNA (32-MER)





● Molecule 7: DNA (5'-D(*TP*GP*CP*TP*CP*TP*CP*AP*GP*CP*CP*GP*CP*AP*AP*GP*GP*AP*CP*CP*GP*CP*AP*TP*AP*CP*TP*AP*CP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.49Å 76.22Å 139.19Å 90.32° 104.83° 118.58°	Depositor
Resolution (Å)	44.34 – 2.10 44.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.34-2.10) 92.8 (44.34-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.208 , 0.246 0.208 , 0.246	Depositor DCC
R_{free} test set	7441 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
Estimated twinning fraction	0.005 for k,-h-k,h+l 0.005 for -h-k,h,h+k+l 0.017 for h,-h-k,-h-l 0.017 for -h-k,k,-l 0.016 for k,h,-h-k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 148843 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19952	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.23	0/4561	0.36	0/6184
2	B	0.24	0/2512	0.39	0/3401
3	C	0.23	0/2445	0.39	0/3320
3	D	0.24	0/2467	0.38	0/3348
3	E	0.24	0/2436	0.38	0/3315
4	F	0.23	0/1131	0.35	0/1527
4	G	0.23	0/1190	0.35	0/1609
5	H	0.24	0/2306	0.35	0/3124
6	I	0.24	0/758	0.84	1/1180 (0.1%)
7	J	0.52	0/503	0.84	0/772
All	All	0.25	0/20309	0.42	1/27780 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	15	U	O4'-C1'-N1	5.16	112.32	108.20

There are no chirality outliers.

There are no planarity outliers.

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	4470	0	4434	23	0
2	B	2458	0	2480	9	0
3	C	2405	0	2362	12	0
3	D	2428	0	2351	14	0
3	E	2395	0	2289	15	0
4	F	1110	0	1097	8	0
4	G	1167	0	1137	10	0
5	H	2260	0	2132	9	0
6	I	679	0	343	5	0
7	J	448	0	245	3	0
8	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	32	0	0	0	0
10	B	23	0	0	0	0
10	C	16	0	0	0	0
10	D	14	0	0	0	0
10	E	13	0	0	0	0
10	G	5	0	0	0	0
10	H	4	0	0	0	0
10	I	23	0	0	0	0
All	All	19952	0	18870	92	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 2.

All (92) 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)
3:E:331:GLY:O	6:I:20:G:N2	2.27	0.68
3:C:201:ILE:HD13	4:F:131:ILE:HG12	1.77	0.66
5:H:29:ILE:HD13	5:H:35:ILE:HB	1.80	0.64
2:B:42:ILE:HD13	2:B:178:ILE:HD11	1.82	0.62
1:A:422:LYS:HB3	2:B:108:PRO:HG3	1.83	0.61
4:G:64:LYS:HB3	4:G:69:VAL:HG21	1.83	0.60
3:E:45:ILE:HB	3:E:128:ALA:HB3	1.84	0.59
3:E:258:SER:HB3	5:H:127:ARG:HH21	1.69	0.57
4:G:66:ILE:HD11	5:H:8:LYS:HB3	1.87	0.57
1:A:864:ILE:HD12	1:A:865:THR:HG23	1.87	0.57
1:A:511:TYR:HB3	1:A:591:PRO:HG3	1.88	0.56
2:B:261:SER:OG	2:B:262:ARG:N	2.38	0.55
3:D:130:ILE:HD13	3:D:291:MET:HG2	1.90	0.54
1:A:444:LYS:HB3	2:B:275:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ALA:HA	1:A:727:LEU:HD23	1.90	0.52
3:D:261:ILE:HG21	4:F:47:LEU:HD21	1.91	0.52
3:E:123:VAL:HG11	3:E:319:LEU:HD11	1.92	0.52
3:E:260:GLU:HB2	3:E:284:PHE:HB2	1.91	0.52
6:I:32:U:H1'	7:J:11:DC:H4'	1.93	0.51
3:C:45:ILE:HB	3:C:128:ALA:HB3	1.92	0.51
3:C:201:ILE:HG12	3:C:206:VAL:HG22	1.93	0.51
2:B:150:LYS:HB3	2:B:162:MET:HB3	1.91	0.51
3:D:135:VAL:HG13	3:D:203:GLU:HG2	1.91	0.51
3:C:130:ILE:HD11	3:C:133:PHE:HB2	1.92	0.50
1:A:448:CYS:HB2	1:A:478:CYS:HB3	1.92	0.50
3:D:329:GLN:HG3	3:D:334:GLU:HG3	1.94	0.50
1:A:820:ARG:HA	1:A:827:THR:HG23	1.93	0.50
3:C:260:GLU:HB2	3:C:284:PHE:HB2	1.94	0.50
1:A:803:PRO:HD3	4:F:11:ALA:HB1	1.93	0.49
1:A:638:THR:HG22	1:A:640:GLN:H	1.78	0.49
3:C:201:ILE:HG21	4:F:131:ILE:HG12	1.93	0.49
5:H:113:LEU:HA	5:H:122:SER:O	2.13	0.48
1:A:845:VAL:HG21	1:A:857:LEU:HB2	1.95	0.47
5:H:29:ILE:HG21	5:H:35:ILE:HD12	1.95	0.47
3:C:181:LEU:HD21	3:C:187:ILE:HG13	1.94	0.47
4:G:41:LYS:HE2	4:G:45:ILE:HD11	1.95	0.47
1:A:722:PRO:HG3	2:B:27:VAL:HG21	1.95	0.47
4:F:67:ASP:HA	4:G:22:LYS:HE2	1.95	0.47
3:D:62:GLU:CD	3:D:102:PRO:HB2	2.35	0.47
5:H:188:ASP:N	5:H:188:ASP:OD1	2.47	0.47
3:D:328:LEU:HD12	3:D:343:VAL:HG21	1.98	0.46
1:A:543:LEU:HD13	1:A:548:LEU:HB2	1.97	0.46
1:A:468:LYS:O	1:A:474:GLU:HA	2.15	0.46
1:A:371:THR:HG22	1:A:431:LYS:HD2	1.98	0.46
5:H:251:GLN:CD	5:H:296:GLU:H	2.20	0.45
4:G:95:SER:HA	4:G:117:PRO:HG2	1.98	0.45
1:A:322:ILE:HD12	1:A:368:VAL:HG21	1.99	0.45
3:C:79:LYS:HA	3:C:82:GLU:HG2	1.99	0.44
3:C:254:PHE:O	3:C:258:SER:HB2	2.16	0.44
3:C:194:LEU:HD21	4:F:127:ILE:HG21	2.00	0.44
4:G:21:ILE:HD11	4:G:93:HIS:HE1	1.82	0.44
3:C:18:PRO:HB2	3:C:338:LYS:HD2	1.98	0.44
3:E:74:TRP:HH2	3:E:306:PRO:HG2	1.83	0.44
2:B:218:ARG:O	2:B:301:PRO:HG3	2.18	0.44
3:E:132:LEU:HB2	3:E:290:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PHE:HD2	2:B:287:SER:HA	1.83	0.44
4:G:141:ASN:O	4:G:145:LYS:HG3	2.18	0.44
1:A:549:TYR:O	1:A:584:TYR:OH	2.32	0.43
6:I:16:A:H2'	6:I:17:U:C6	2.53	0.43
1:A:521:LYS:HB3	1:A:522:TYR:CD2	2.53	0.43
3:E:32:LEU:HD12	3:E:282:GLU:HG2	2.00	0.43
3:D:123:VAL:HG11	3:D:319:LEU:HD11	2.01	0.43
1:A:338:VAL:HG21	1:A:350:LYS:HG2	1.99	0.43
3:D:181:LEU:HD21	3:D:187:ILE:HG13	2.00	0.43
6:I:12:U:O4	6:I:13:A:N6	2.52	0.43
4:G:60:SER:HB2	5:H:50:TYR:O	2.17	0.43
1:A:531:ARG:HB2	1:A:538:VAL:HG21	2.00	0.43
3:E:329:GLN:OE1	6:I:20:G:N2	2.46	0.42
7:J:10:DC:H2'	7:J:11:DC:H6	1.84	0.42
4:G:99:ALA:HA	4:G:112:THR:OG1	2.19	0.42
3:D:132:LEU:HB2	3:D:290:LEU:HB3	2.02	0.42
3:D:19:VAL:HG22	3:D:339:GLY:HA2	2.01	0.42
4:F:120:TYR:CE1	4:F:124:LYS:HG3	2.55	0.42
1:A:252:LEU:HD22	1:A:322:ILE:HG23	2.01	0.42
2:B:35:PRO:HB2	2:B:311:LEU:O	2.20	0.42
3:E:203:GLU:HG3	3:E:258:SER:OG	2.20	0.42
1:A:531:ARG:HG3	1:A:535:GLU:HA	2.01	0.41
3:E:201:ILE:HG12	3:E:206:VAL:HG22	2.03	0.41
5:H:112:GLY:HA3	5:H:124:ARG:HG2	2.02	0.41
3:E:134:PRO:HG2	3:E:286:PRO:HG2	2.03	0.41
7:J:10:DC:H2'	7:J:11:DC:C6	2.56	0.41
3:C:263:ALA:HB2	3:C:281:TYR:CE1	2.56	0.41
3:E:249:ASP:HB3	4:G:127:ILE:HD12	2.02	0.41
3:D:14:TYR:CZ	3:D:288:ASP:HA	2.56	0.40
4:F:81:ASN:OD1	4:F:81:ASN:N	2.53	0.40
1:A:509:LEU:HA	1:A:591:PRO:HG2	2.03	0.40
3:D:6:GLU:HB2	3:D:312:THR:HG21	2.02	0.40
1:A:486:TYR:O	1:A:489:VAL:HG22	2.22	0.40
3:E:329:GLN:HG3	3:E:334:GLU:HG3	2.03	0.40
3:D:14:TYR:CE1	3:D:234:LYS:HE3	2.56	0.40
3:E:8:ALA:HB3	3:E:161:VAL:HG13	2.03	0.40
3:D:27:LEU:HD23	3:D:27:LEU:HA	1.92	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	559/677 (83%)	551 (99%)	8 (1%)	0	100	100
2	B	315/322 (98%)	304 (96%)	11 (4%)	0	100	100
3	C	316/357 (88%)	309 (98%)	7 (2%)	0	100	100
3	D	319/357 (89%)	310 (97%)	9 (3%)	0	100	100
3	E	322/357 (90%)	313 (97%)	9 (3%)	0	100	100
4	F	142/155 (92%)	141 (99%)	1 (1%)	0	100	100
4	G	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
5	H	291/349 (83%)	283 (97%)	7 (2%)	1 (0%)	46	45
All	All	2414/2729 (88%)	2354 (98%)	59 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	217	ILE

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	457/604 (76%)	456 (100%)	1 (0%)	95	97
2	B	257/280 (92%)	256 (100%)	1 (0%)	93	96
3	C	243/309 (79%)	242 (100%)	1 (0%)	93	96
3	D	238/309 (77%)	237 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	228/309 (74%)	225 (99%)	3 (1%)	76	82
4	F	111/131 (85%)	111 (100%)	0	100	100
4	G	119/131 (91%)	119 (100%)	0	100	100
5	H	224/309 (72%)	223 (100%)	1 (0%)	93	96
All	All	1877/2382 (79%)	1869 (100%)	8 (0%)	93	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	VAL
2	B	2	ILE
3	C	39	HIS
3	D	2	PHE
3	E	229	ASP
3	E	268	ASP
3	E	338	LYS
5	H	89	TYR

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	I	31/39 (79%)	3 (9%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	I	2	U
6	I	14	G
6	I	27	G

There are no RNA pucker outliers to report.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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(Å ²)	Q<0.9
1	A	573/677 (84%)	0.19	26 (4%) 37 46	21, 35, 58, 65	0
2	B	319/322 (99%)	0.12	2 (0%) 90 92	21, 33, 51, 64	0
3	C	322/357 (90%)	0.16	3 (0%) 85 88	21, 34, 52, 65	0
3	D	331/357 (92%)	0.38	15 (4%) 37 46	23, 37, 64, 81	0
3	E	330/357 (92%)	0.67	35 (10%) 8 11	25, 39, 64, 77	0
4	F	146/155 (94%)	0.27	8 (5%) 29 37	24, 37, 60, 72	0
4	G	152/155 (98%)	0.19	9 (5%) 26 34	24, 35, 52, 61	0
5	H	297/349 (85%)	0.36	24 (8%) 15 20	25, 39, 68, 77	0
6	I	32/39 (82%)	-0.25	2 (6%) 23 31	25, 29, 61, 79	0
7	J	22/31 (70%)	-0.20	0 100 100	32, 46, 60, 62	0
All	All	2524/2799 (90%)	0.28	124 (4%) 33 42	21, 36, 61, 81	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	228	GLY	5.7
1	A	527	VAL	5.2
5	H	219	ASP	5.1
3	D	179	VAL	5.0
2	B	50	GLY	4.9
5	H	191	LEU	4.7
1	A	830	LEU	4.7
1	A	536	ASP	4.7
5	H	190	TYR	4.6
1	A	579	PHE	4.3
3	E	213	SER	4.3
5	H	189	TYR	4.3
5	H	218	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
3	E	80	THR	4.0
3	E	312	THR	3.9
3	E	309	VAL	3.8
3	D	233	GLY	3.8
1	A	382	TYR	3.7
5	H	161	ARG	3.7
5	H	188	ASP	3.7
4	F	104	LYS	3.6
3	E	91	PHE	3.5
3	E	179	VAL	3.5
5	H	210	ILE	3.5
4	G	152	GLU	3.5
1	A	544	VAL	3.5
3	E	74	TRP	3.4
4	F	105	ASP	3.4
3	E	63	LEU	3.3
4	G	81	ASN	3.3
1	A	381	ILE	3.3
1	A	699	PHE	3.2
3	E	83	VAL	3.2
4	F	103	GLY	3.2
5	H	209	ALA	3.1
5	H	208	GLY	3.1
1	A	410	VAL	3.1
1	A	462	TYR	3.1
1	A	541	ASN	3.1
1	A	587	ILE	3.1
3	D	170	LEU	3.0
5	H	170	LEU	3.0
1	A	531	ARG	3.0
4	F	81	ASN	3.0
4	F	79	PHE	3.0
3	D	196	GLY	2.9
4	F	80	GLY	2.9
1	A	538	VAL	2.9
3	D	225	THR	2.8
3	E	76	TRP	2.8
3	E	306	PRO	2.8
1	A	346	ASP	2.8
3	E	224	LYS	2.8
3	E	5	PHE	2.7
1	A	530	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	273	THR	2.7
3	C	233	GLY	2.7
3	E	158	PHE	2.7
3	E	305	LEU	2.6
5	H	195	VAL	2.6
5	H	207	LEU	2.6
1	A	826	GLU	2.6
3	E	32	LEU	2.6
3	E	261	ILE	2.6
4	F	77	GLU	2.6
1	A	540	ASP	2.6
3	E	166	ASN	2.5
4	G	153	GLU	2.5
3	D	227	PHE	2.5
3	E	25	ALA	2.5
5	H	194	ALA	2.5
3	E	33	PRO	2.5
4	G	80	GLY	2.5
6	I	31	C	2.5
2	B	53	ASN	2.5
5	H	166	VAL	2.5
5	H	168	GLU	2.4
1	A	573	VAL	2.4
3	E	4	MET	2.4
3	E	34	ILE	2.4
4	G	78	SER	2.4
3	E	214	ASN	2.4
3	E	284	PHE	2.4
3	E	211	SER	2.4
3	E	259	THR	2.4
5	H	332	LEU	2.4
3	E	195	ASN	2.4
4	G	82	ALA	2.3
3	E	114	ASP	2.3
3	D	1	MET	2.3
4	F	66	ILE	2.3
3	D	81	LYS	2.3
5	H	150	ILE	2.3
3	D	169	GLU	2.3
5	H	193	ALA	2.3
1	A	542	MET	2.2
1	A	349	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	539	LYS	2.2
4	G	27	GLN	2.2
1	A	347	ARG	2.2
3	E	120	ALA	2.2
1	A	409	ARG	2.2
1	A	351	ASP	2.2
3	D	285	LEU	2.2
5	H	160	LEU	2.2
4	G	105	ASP	2.2
4	G	77	GLU	2.2
3	D	229	ASP	2.1
3	E	21	ALA	2.1
6	I	32	U	2.1
3	E	103	LEU	2.1
3	E	96	GLU	2.1
5	H	169	ASP	2.1
5	H	165	SER	2.1
3	D	261	ILE	2.1
5	H	159	ILE	2.1
3	D	167	ASP	2.1
3	C	235	PRO	2.0
3	E	27	LEU	2.0
1	A	576	VAL	2.0
3	E	220	VAL	2.0
3	D	262	VAL	2.0
5	H	221	VAL	2.0
3	C	229	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
8	ZN	A	901	1/1	1.00	0.12	0.06	30,30,30,30	0
9	MG	B	401	1/1	0.98	0.10	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.