



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:32 am BST

PDB ID : 4LEY
Title : Structure of mouse cGAS bound to 18 bp DNA
Authors : Li, P.
Deposited on : 2013-06-26
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

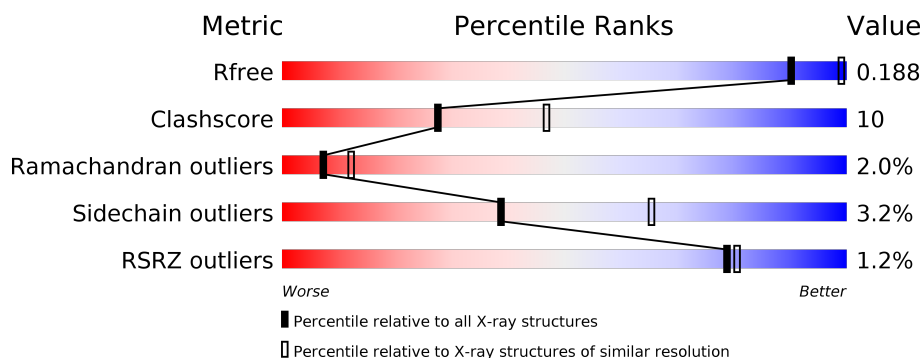
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	366	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	366	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
1	C	366	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• • •</div> </div> </div>
1	D	366	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>• •</div> </div> </div>
2	E	18	<div> <div></div> <div> <div>56%</div> <div>39%</div> <div>6%</div> </div> </div>
2	F	18	<div> <div></div> <div> <div>83%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	18	 56% 39% 6%
2	H	18	 67% 33%
2	I	18	 56% 44%
2	J	18	 89% 11%
2	K	18	 83% 11% 6%
2	L	18	 94% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15439 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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2969	1910	506	540	13			
1	B	359	Total	C	N	O	S	0	0	0
			2969	1910	506	540	13			
1	C	359	Total	C	N	O	S	0	0	0
			2969	1910	506	540	13			
1	D	359	Total	C	N	O	S	0	0	0
			2969	1910	506	540	13			

- Molecule 2 is a DNA chain called 18 bp dsDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	F	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	G	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	H	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	I	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	J	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	K	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	L	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

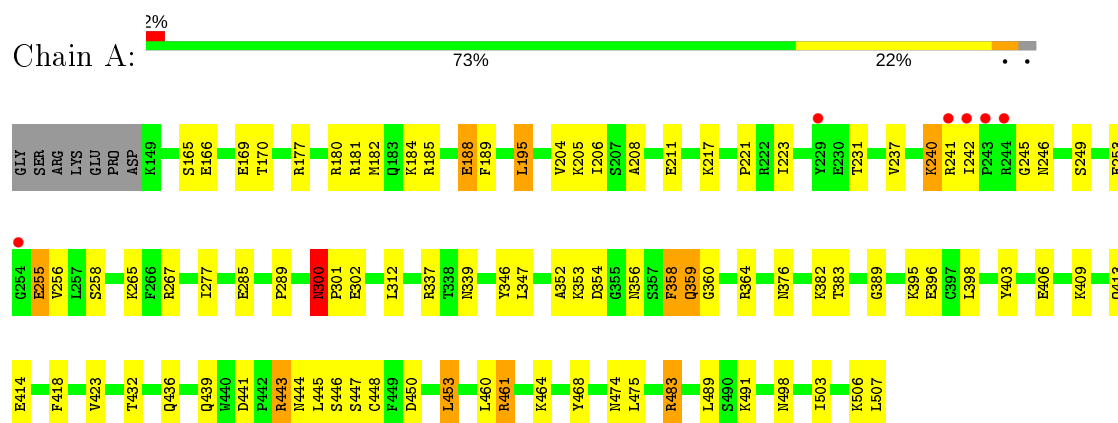
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	127	Total O 127 127	0	0
4	B	120	Total O 120 120	0	0
4	C	129	Total O 129 129	0	0
4	D	132	Total O 132 132	0	0
4	E	19	Total O 19 19	0	0
4	F	14	Total O 14 14	0	0
4	G	17	Total O 17 17	0	0
4	H	12	Total O 12 12	0	0
4	I	21	Total O 21 21	0	0
4	J	10	Total O 10 10	0	0
4	K	12	Total O 12 12	0	0
4	L	18	Total O 18 18	0	0

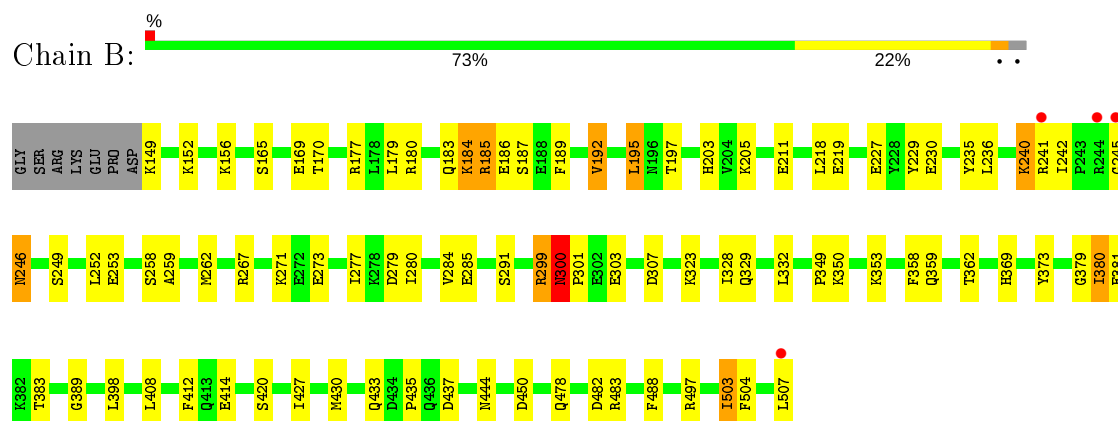
3 Residue-property plots

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

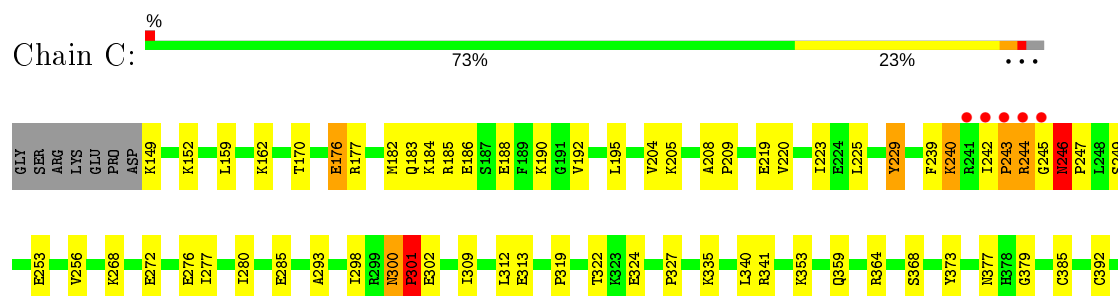
• Molecule 1: Cyclic GMP-AMP synthase



• Molecule 1: Cyclic GMP-AMP synthase

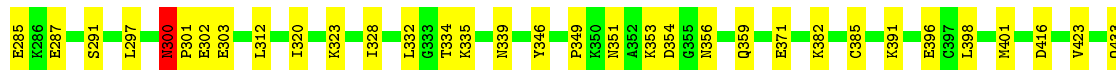
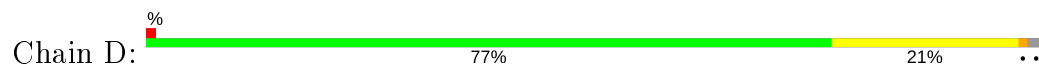


• Molecule 1: Cyclic GMP-AMP synthase





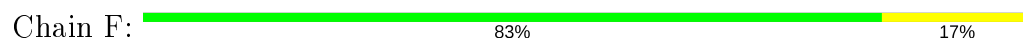
- Molecule 1: Cyclic GMP-AMP synthase



- Molecule 2: 18 bp dsDNA



- Molecule 2: 18 bp dsDNA



- Molecule 2: 18 bp dsDNA

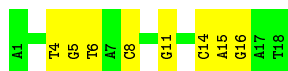


- Molecule 2: 18 bp dsDNA



- Molecule 2: 18 bp dsDNA





- Molecule 2: 18 bp dsDNA

Chain J: 89% 11%



- Molecule 2: 18 bp dsDNA

Chain K: 83% 11% 6%



- Molecule 2: 18 bp dsDNA

Chain L: 94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.38 Å 145.90 Å 100.96 Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	40.77 – 2.50 40.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.77-2.50) 96.1 (40.77-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.51 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.161 , 0.191 0.153 , 0.188	Depositor DCC
R_{free} test set	1993 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 16.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.416 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15439	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ZN

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	0.29	0/3033	0.47	0/4071
1	B	0.29	0/3033	0.45	0/4071
1	C	0.29	0/3033	0.47	0/4071
1	D	0.29	0/3033	0.45	0/4071
2	E	0.49	0/410	1.31	2/631 (0.3%)
2	F	0.47	0/410	1.24	0/631
2	G	0.50	0/410	1.30	2/631 (0.3%)
2	H	0.49	0/410	1.26	4/631 (0.6%)
2	I	0.48	0/410	1.32	1/631 (0.2%)
2	J	0.47	0/410	1.20	0/631
2	K	0.49	0/410	1.35	2/631 (0.3%)
2	L	0.50	0/410	1.21	0/631
All	All	0.34	0/15412	0.74	11/21332 (0.1%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7	DA	O4'-C1'-N9	7.24	113.06	108.00
2	G	8	DC	O4'-C1'-N1	7.14	113.00	108.00
2	H	14	DC	O4'-C1'-N1	7.00	112.90	108.00
2	K	7	DA	O4'-C1'-N9	6.72	112.71	108.00
2	H	9	DA	O4'-C1'-N9	6.05	112.23	108.00
2	E	15	DA	O4'-C1'-N9	5.91	112.14	108.00
2	K	13	DA	O4'-C1'-N9	5.82	112.08	108.00
2	I	8	DC	O4'-C1'-N1	5.72	112.00	108.00
2	H	16	DG	O4'-C1'-N9	5.57	111.90	108.00
2	G	3	DC	O4'-C1'-N1	5.52	111.87	108.00
2	H	8	DC	C1'-O4'-C4'	-5.00	105.10	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	ASN	Peptide
1	B	300	ASN	Peptide
1	C	300	ASN	Peptide
1	D	300	ASN	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	2969	0	3022	65	0
1	B	2969	0	3022	58	0
1	C	2969	0	3022	58	0
1	D	2969	0	3022	54	0
2	E	366	0	206	7	0
2	F	366	0	206	2	0
2	G	366	0	206	9	0
2	H	366	0	206	2	0
2	I	366	0	206	10	0
2	J	366	0	206	2	0
2	K	366	0	206	2	0
2	L	366	0	206	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	127	0	0	24	0
4	B	120	0	0	17	0
4	C	129	0	0	19	0
4	D	132	0	0	17	0
4	E	19	0	0	2	0
4	F	14	0	0	2	0
4	G	17	0	0	6	0
4	H	12	0	0	1	0
4	I	21	0	0	7	0
4	J	10	0	0	1	0
4	K	12	0	0	1	0
4	L	18	0	0	2	0
All	All	15439	0	13736	260	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 (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:ND2	4:A:788:HOH:O	1.99	0.95
1:A:166:GLU:OE1	4:A:794:HOH:O	1.88	0.92
2:G:10:DT:OP2	4:G:115:HOH:O	1.88	0.91
1:C:392:CYS:SG	4:C:713:HOH:O	2.29	0.90
1:B:350:LYS:O	4:B:725:HOH:O	1.90	0.90
1:C:285:GLU:OE1	4:C:744:HOH:O	1.91	0.89
1:D:291:SER:O	4:D:740:HOH:O	1.92	0.87
1:B:203:HIS:ND1	4:B:759:HOH:O	2.09	0.86
1:C:176:GLU:OE2	4:C:753:HOH:O	1.93	0.86
1:A:302:GLU:OE2	4:A:770:HOH:O	1.95	0.85
1:D:323:LYS:NZ	4:D:781:HOH:O	2.08	0.85
1:A:441:ASP:OD2	4:A:762:HOH:O	1.94	0.84
1:C:368:SER:O	4:C:794:HOH:O	1.94	0.84
1:C:341:ARG:O	4:C:745:HOH:O	1.96	0.84
1:A:352:ALA:O	4:A:734:HOH:O	1.95	0.83
1:A:339:ASN:O	4:A:724:HOH:O	1.97	0.81
1:D:267:ARG:NH1	4:D:729:HOH:O	2.14	0.80
1:B:245:GLY:O	1:B:249:SER:OG	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ASN:ND2	4:C:808:HOH:O	2.14	0.79
1:B:291:SER:O	4:B:756:HOH:O	2.00	0.78
1:D:152:LYS:O	4:D:719:HOH:O	2.02	0.76
1:D:285:GLU:OE1	4:D:734:HOH:O	2.02	0.76
1:D:183:GLN:NE2	1:D:192:VAL:O	2.19	0.76
1:B:420:SER:OG	4:B:804:HOH:O	2.04	0.75
1:B:169:GLU:OE2	4:B:779:HOH:O	2.04	0.74
1:A:359:GLN:O	4:A:786:HOH:O	2.04	0.74
1:C:183:GLN:OE1	4:C:821:HOH:O	2.06	0.74
1:A:211:GLU:OE2	4:A:741:HOH:O	2.04	0.74
1:D:371:GLU:OE1	4:D:724:HOH:O	2.04	0.73
1:A:432:THR:OG1	1:A:468:TYR:OH	2.07	0.73
2:I:14:DC:OP1	4:I:108:HOH:O	2.06	0.73
2:I:5:DG:OP1	4:I:101:HOH:O	2.05	0.73
1:D:416:ASP:OD1	4:D:733:HOH:O	2.07	0.73
1:A:364:ARG:NH1	4:A:705:HOH:O	2.22	0.72
1:A:267:ARG:NH2	1:A:285:GLU:O	2.22	0.72
1:D:339:ASN:O	4:D:799:HOH:O	2.08	0.71
2:G:16:DG:OP2	4:G:116:HOH:O	2.07	0.71
1:D:185:ARG:NH2	4:D:824:HOH:O	2.22	0.71
2:I:6:DT:OP1	4:I:107:HOH:O	2.08	0.71
1:B:279:ASP:OD1	4:B:723:HOH:O	2.08	0.71
1:B:156:LYS:NZ	1:B:504:PHE:O	2.23	0.70
1:B:379:GLY:O	1:D:382:LYS:NZ	2.26	0.69
1:B:478:GLN:NE2	1:B:482:ASP:OD1	2.26	0.69
1:D:481:ILE:O	1:D:486:LYS:NZ	2.25	0.69
1:A:245:GLY:O	1:A:249:SER:OG	2.10	0.69
1:D:463:GLU:HG2	1:D:486:LYS:HE3	1.74	0.69
1:C:353:LYS:HA	1:C:359:GLN:HE21	1.59	0.67
1:C:490:SER:N	4:C:804:HOH:O	2.19	0.67
2:I:5:DG:N2	4:I:113:HOH:O	2.20	0.67
1:C:184:LYS:O	1:C:186:GLU:N	2.25	0.67
1:D:149:LYS:N	4:D:785:HOH:O	2.28	0.67
1:C:324:GLU:OE1	4:C:712:HOH:O	2.13	0.66
1:A:406:GLU:OE2	4:A:704:HOH:O	2.13	0.66
1:A:358:PHE:O	1:A:360:GLY:N	2.28	0.66
1:A:376:ASN:OD1	4:A:708:HOH:O	2.12	0.65
1:B:381:GLU:OE1	4:B:810:HOH:O	2.13	0.65
2:I:4:DT:O2	4:I:109:HOH:O	2.09	0.65
1:C:377:ASN:OD1	4:C:725:HOH:O	2.15	0.65
2:E:10:DT:OP2	4:E:117:HOH:O	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:DG:O6	4:E:101:HOH:O	2.11	0.65
1:C:464:LYS:NZ	1:C:466:ASP:OD2	2.29	0.65
1:B:307:ASP:OD2	4:B:748:HOH:O	2.15	0.64
2:F:10:DT:O4	4:F:114:HOH:O	2.14	0.64
1:D:302:GLU:OE1	4:D:736:HOH:O	2.15	0.64
1:A:356:ASN:OD1	4:A:795:HOH:O	2.15	0.64
1:B:267:ARG:NH2	1:B:285:GLU:O	2.31	0.64
2:G:16:DG:N7	4:G:103:HOH:O	2.30	0.64
1:B:170:THR:HG23	1:B:280:ILE:HD12	1.80	0.64
1:A:444:ASN:ND2	1:A:448:CYS:SG	2.66	0.63
1:D:238:LYS:HB3	1:D:255:GLU:HG2	1.81	0.63
1:A:289:PRO:HD3	4:A:792:HOH:O	1.99	0.63
1:C:162:LYS:NZ	4:C:752:HOH:O	2.33	0.62
1:A:444:ASN:O	1:A:446:SER:N	2.33	0.62
1:C:240:LYS:HA	4:C:805:HOH:O	1.99	0.61
1:D:170:THR:HG23	1:D:280:ILE:HD12	1.82	0.61
1:C:300:ASN:O	1:C:302:GLU:N	2.33	0.61
1:C:503:ILE:HG13	1:C:506:LYS:HE2	1.82	0.61
1:D:244:ARG:HH12	1:D:247:PRO:HD3	1.65	0.61
1:A:188:GLU:OE2	1:A:265:LYS:NZ	2.30	0.61
2:H:12:DT:OP2	4:H:108:HOH:O	2.15	0.60
1:C:298:ILE:HG22	1:C:300:ASN:H	1.67	0.60
2:L:4:DT:O2	4:L:109:HOH:O	2.15	0.60
1:D:287:GLU:OE2	1:D:351:ASN:ND2	2.32	0.60
1:A:409:LYS:NZ	1:A:418:PHE:O	2.23	0.59
1:B:414:GLU:N	1:B:414:GLU:OE2	2.33	0.59
1:A:413:GLN:NE2	4:A:779:HOH:O	2.27	0.59
1:A:302:GLU:HB3	4:A:770:HOH:O	2.03	0.58
1:A:436:GLN:HB2	1:A:439:GLN:HG3	1.83	0.58
1:A:444:ASN:HD22	1:A:448:CYS:H	1.50	0.58
1:C:170:THR:HG23	1:C:280:ILE:HD12	1.85	0.58
1:A:204:VAL:HG11	1:A:398:LEU:HD23	1.84	0.58
1:A:170:THR:OG1	1:A:300:ASN:ND2	2.37	0.58
1:C:246:ASN:O	1:C:249:SER:OG	2.20	0.58
1:C:220:VAL:HG21	1:C:312:LEU:HD22	1.84	0.58
1:A:337:ARG:NH1	4:A:709:HOH:O	2.06	0.57
1:A:383:THR:O	1:A:389:GLY:HA3	2.05	0.57
1:A:444:ASN:ND2	1:A:448:CYS:H	2.03	0.57
1:C:245:GLY:O	1:C:249:SER:OG	2.22	0.57
1:A:205:LYS:NZ	1:A:208:ALA:O	2.36	0.56
1:A:255:GLU:HG3	1:A:256:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLU:OE2	1:A:414:GLU:N	2.37	0.56
1:D:220:VAL:HG21	1:D:312:LEU:HD22	1.86	0.56
1:D:448:CYS:O	1:D:451:LYS:HG2	2.05	0.56
1:B:373:TYR:OH	4:B:732:HOH:O	2.15	0.56
1:A:460:LEU:HD21	1:A:489:LEU:HD23	1.87	0.56
1:A:483:ARG:HH12	1:D:438:SER:HA	1.70	0.55
1:C:177:ARG:NH2	1:C:276:GLU:O	2.39	0.55
1:A:503:ILE:HG13	1:A:506:LYS:HD2	1.89	0.55
1:C:481:ILE:O	1:C:486:LYS:NZ	2.33	0.55
1:C:186:GLU:OE2	1:C:190:LYS:NZ	2.40	0.55
1:B:450:ASP:OD1	1:B:497:ARG:NH2	2.39	0.55
1:B:353:LYS:HA	1:B:359:GLN:HE21	1.72	0.54
2:I:5:DG:O6	2:J:13:DA:N6	2.40	0.54
1:B:219:GLU:OE1	4:B:743:HOH:O	2.18	0.54
1:D:353:LYS:HA	1:D:359:GLN:NE2	2.23	0.54
1:A:253:GLU:HB2	1:A:258:SER:HB2	1.90	0.54
1:B:358:PHE:O	1:B:362:THR:OG1	2.25	0.54
1:C:463:GLU:HG2	1:C:486:LYS:HE3	1.89	0.54
1:B:246:ASN:O	1:B:249:SER:OG	2.25	0.53
1:A:395:LYS:NZ	4:A:708:HOH:O	2.34	0.53
1:B:170:THR:OG1	1:B:300:ASN:ND2	2.42	0.53
1:D:183:GLN:HG3	1:D:191:GLY:H	1.73	0.53
2:J:1:DA:H3'	4:J:107:HOH:O	2.08	0.53
2:E:1:DA:HO5'	2:E:1:DA:H8	1.55	0.53
1:D:494:GLU:HG3	4:D:753:HOH:O	2.09	0.53
2:I:11:DG:H4'	4:I:111:HOH:O	2.09	0.53
1:C:249:SER:N	4:C:806:HOH:O	2.42	0.52
1:C:319:PRO:O	1:C:322:THR:OG1	2.26	0.52
2:L:4:DT:H1'	4:L:109:HOH:O	2.09	0.52
1:D:180:ARG:NH2	2:K:7:DA:OP1	2.43	0.51
2:G:5:DG:N3	4:G:106:HOH:O	2.33	0.51
1:D:328:ILE:HB	1:D:332:LEU:HB2	1.92	0.51
1:A:165:SER:O	1:A:169:GLU:HG3	2.11	0.51
1:B:229:TYR:O	4:B:770:HOH:O	2.19	0.51
1:B:253:GLU:HG3	1:B:258:SER:HB2	1.91	0.51
2:K:5:DG:O6	4:K:107:HOH:O	2.18	0.51
1:A:444:ASN:HB2	1:A:447:SER:HB3	1.91	0.51
1:C:247:PRO:O	4:C:806:HOH:O	2.20	0.51
1:C:433:GLN:O	1:C:435:PRO:HD3	2.11	0.51
1:D:453:LEU:HD23	1:D:497:ARG:HD3	1.93	0.51
1:A:483:ARG:NH2	4:A:784:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:DG:N7	4:I:103:HOH:O	2.34	0.50
1:B:271:LYS:HG2	1:B:284:VAL:HG21	1.92	0.50
1:C:407:GLN:HB3	1:C:503:ILE:HG12	1.92	0.50
1:B:478:GLN:OE1	1:B:483:ARG:HG3	2.12	0.50
1:D:487:GLU:O	1:D:491:LYS:HG2	2.11	0.50
1:C:465:LEU:O	1:C:475:LEU:HB2	2.11	0.50
1:A:353:LYS:HA	1:A:359:GLN:HE21	1.77	0.49
1:A:464:LYS:HA	1:A:474:ASN:HD21	1.76	0.49
1:B:408:LEU:HD23	1:B:503:ILE:HD13	1.93	0.49
1:D:204:VAL:HG11	1:D:398:LEU:HD23	1.93	0.49
1:A:483:ARG:NE	4:A:784:HOH:O	2.45	0.49
1:B:299:ARG:HD2	1:B:303:GLU:HG2	1.94	0.49
1:C:219:GLU:HA	1:C:313:GLU:HB3	1.94	0.48
1:D:436:GLN:HB2	1:D:439:GLN:HG3	1.95	0.48
1:A:180:ARG:NE	4:A:800:HOH:O	2.45	0.48
1:B:383:THR:O	1:B:389:GLY:HA3	2.14	0.48
1:C:149:LYS:N	1:C:152:LYS:HE3	2.28	0.48
2:I:14:DC:H2''	2:I:15:DA:C8	2.48	0.48
1:A:177:ARG:HD3	1:A:277:ILE:HG12	1.95	0.47
1:A:461:ARG:NH2	4:A:702:HOH:O	2.18	0.47
2:G:3:DC:H5'	4:G:111:HOH:O	2.14	0.47
1:B:273:GLU:OE1	4:B:814:HOH:O	2.20	0.47
1:A:195:LEU:HD12	1:A:217:LYS:HD3	1.95	0.47
1:A:177:ARG:NH1	4:A:804:HOH:O	2.29	0.47
1:B:179:LEU:O	1:B:183:GLN:HG2	2.15	0.47
1:A:395:LYS:NZ	2:E:15:DA:OP1	2.35	0.47
1:C:268:LYS:NZ	1:C:272:GLU:OE1	2.40	0.47
1:A:312:LEU:HB2	1:A:347:LEU:HB2	1.96	0.46
1:D:177:ARG:NH1	4:D:751:HOH:O	2.29	0.46
1:D:195:LEU:HD12	1:D:217:LYS:HD3	1.97	0.46
2:G:7:DA:OP2	4:G:108:HOH:O	2.20	0.46
2:I:15:DA:H2''	2:I:16:DG:H8	1.80	0.46
1:D:280:ILE:O	4:D:768:HOH:O	2.20	0.46
1:D:300:ASN:O	1:D:302:GLU:HG2	2.15	0.46
1:D:335:LYS:HG2	2:G:9:DA:H4'	1.97	0.46
1:A:217:LYS:HD2	1:A:346:TYR:HE2	1.81	0.46
2:E:1:DA:H2'	2:E:2:DT:C6	2.50	0.46
1:A:188:GLU:H	1:A:188:GLU:HG2	1.50	0.46
1:C:204:VAL:HG21	1:C:398:LEU:HD23	1.97	0.46
1:A:182:MET:HG3	1:A:189:PHE:HB2	1.97	0.45
1:A:217:LYS:HD2	1:A:346:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ARG:NH2	1:B:273:GLU:OE2	2.36	0.45
1:C:293:ALA:HB2	1:C:309:ILE:HG12	1.98	0.45
1:A:181:ARG:CZ	1:A:185:ARG:HD3	2.46	0.45
1:A:382:LYS:NZ	1:C:379:GLY:O	2.34	0.45
2:F:4:DT:H2"	2:F:5:DG:C8	2.52	0.45
1:A:450:ASP:HA	1:A:453:LEU:HD22	1.99	0.45
1:A:491:LYS:HG2	1:B:435:PRO:HG2	1.99	0.45
1:B:185:ARG:O	1:B:187:SER:N	2.50	0.45
1:C:385:CYS:HB2	4:C:813:HOH:O	2.17	0.45
1:D:149:LYS:HE2	1:D:446:SER:OG	2.17	0.45
1:C:340:LEU:HD21	1:C:373:TYR:CD1	2.52	0.45
1:C:327:PRO:HD2	1:C:468:TYR:CZ	2.52	0.45
1:D:259:ALA:HB1	1:D:349:PRO:HB3	1.99	0.45
1:C:335:LYS:HG2	2:E:13:DA:H4'	1.99	0.44
1:B:205:LYS:HE2	1:B:211:GLU:HB2	1.99	0.44
1:B:165:SER:OG	2:H:10:DT:OP1	2.29	0.44
1:D:230:GLU:HB3	4:D:825:HOH:O	2.15	0.44
1:A:206:ILE:O	1:A:208:ALA:N	2.47	0.44
1:B:240:LYS:O	1:B:242:ILE:N	2.51	0.44
1:B:259:ALA:HB1	1:B:349:PRO:HB3	1.99	0.44
1:C:205:LYS:NZ	1:C:208:ALA:O	2.46	0.44
1:B:230:GLU:N	4:B:738:HOH:O	2.24	0.44
1:B:227:GLU:HA	1:B:235:TYR:CD1	2.53	0.44
1:D:243:PRO:HG2	1:D:244:ARG:HG2	2.00	0.44
1:B:328:ILE:HD12	1:B:332:LEU:HB2	2.00	0.43
1:D:385:CYS:SG	1:D:391:LYS:HD2	2.58	0.43
1:D:391:LYS:NZ	1:D:396:GLU:OE2	2.46	0.43
1:B:195:LEU:HD11	1:B:369:HIS:HB3	2.00	0.43
1:C:301:PRO:HD2	4:C:808:HOH:O	2.19	0.43
1:C:436:GLN:HB2	1:C:439:GLN:HG3	2.00	0.43
1:C:473:PHE:HD1	4:C:818:HOH:O	2.01	0.43
1:B:277:ILE:HG23	4:B:723:HOH:O	2.18	0.43
1:D:183:GLN:HA	1:D:190:LYS:HA	2.00	0.43
1:B:180:ARG:HE	1:B:184:LYS:NZ	2.17	0.43
1:B:249:SER:HA	1:B:252:LEU:HD12	2.00	0.43
1:B:177:ARG:HD3	1:B:277:ILE:HG12	2.01	0.43
1:D:334:THR:HB	2:G:9:DA:OP1	2.19	0.43
1:B:323:LYS:NZ	4:B:763:HOH:O	2.51	0.42
1:C:364:ARG:NH2	4:C:777:HOH:O	2.52	0.42
1:B:412:PHE:CD1	1:B:488:PHE:HZ	2.36	0.42
1:C:246:ASN:HA	1:C:247:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HG13	1:A:237:VAL:HG13	2.01	0.42
1:A:240:LYS:HB3	1:A:241:ARG:H	1.57	0.42
1:C:243:PRO:HB2	1:C:244:ARG:H	1.60	0.42
1:C:415:LEU:HD21	1:C:488:PHE:HD2	1.84	0.42
1:C:488:PHE:O	1:C:492:LYS:HG2	2.19	0.42
1:C:242:ILE:HA	1:C:243:PRO:HD3	1.81	0.42
1:B:380:ILE:HD11	1:B:437:ASP:H	1.84	0.42
1:B:184:LYS:HB3	1:B:185:ARG:H	1.64	0.42
1:D:282:VAL:HA	1:D:297:LEU:O	2.20	0.42
1:B:197:THR:HB	4:B:772:HOH:O	2.20	0.42
1:D:465:LEU:N	1:D:474:ASN:OD1	2.47	0.42
1:B:433:GLN:O	1:B:435:PRO:HD3	2.19	0.42
1:B:267:ARG:HG2	1:B:271:LYS:HE3	2.02	0.41
1:B:189:PHE:O	1:B:192:VAL:HB	2.20	0.41
1:C:182:MET:HG2	1:C:192:VAL:HG11	2.02	0.41
1:C:208:ALA:HA	1:C:209:PRO:HD3	1.91	0.41
1:A:205:LYS:HD2	4:A:773:HOH:O	2.20	0.41
1:D:433:GLN:O	1:D:435:PRO:HD3	2.21	0.41
2:G:15:DA:H2"	2:G:16:DG:C8	2.56	0.41
1:A:443:ARG:NE	1:A:444:ASN:OD1	2.54	0.41
1:C:159:LEU:HA	4:C:810:HOH:O	2.19	0.41
1:C:418:PHE:HA	1:C:422:HIS:CE1	2.56	0.41
1:D:217:LYS:HD2	1:D:346:TYR:HE2	1.85	0.41
1:D:494:GLU:CG	4:D:753:HOH:O	2.69	0.40
2:E:18:DT:H1'	4:F:101:HOH:O	2.21	0.40
1:A:403:TYR:OH	4:A:756:HOH:O	2.21	0.40
1:D:472:LYS:HG2	4:D:721:HOH:O	2.21	0.40
1:C:223:ILE:HG22	1:C:239:PHE:CE1	2.57	0.40
1:D:300:ASN:HD22	1:D:300:ASN:HA	1.57	0.40
1:D:401:MET:HG2	1:D:423:VAL:HB	2.02	0.40
1:B:149:LYS:N	1:B:152:LYS:HE3	2.36	0.40
1:B:192:VAL:HG23	1:B:218:LEU:HB2	2.03	0.40
1:B:398:LEU:HD13	1:B:427:ILE:HG21	2.02	0.40
1:B:444:ASN:ND2	4:B:754:HOH:O	2.54	0.40
1:C:253:GLU:HB2	1:C:256:VAL:HG13	2.02	0.40
1:D:267:ARG:NH2	1:D:285:GLU:O	2.54	0.40
1:D:356:ASN:O	1:D:359:GLN:HB2	2.20	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	357/366 (98%)	330 (92%)	17 (5%)	10 (3%)	5	7
1	B	357/366 (98%)	334 (94%)	15 (4%)	8 (2%)	6	10
1	C	357/366 (98%)	331 (93%)	19 (5%)	7 (2%)	7	12
1	D	357/366 (98%)	340 (95%)	14 (4%)	3 (1%)	19	35
All	All	1428/1464 (98%)	1335 (94%)	65 (5%)	28 (2%)	7	12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	240	LYS
1	A	301	PRO
1	B	184	LYS
1	B	186	GLU
1	B	300	ASN
1	B	301	PRO
1	C	185	ARG
1	C	240	LYS
1	C	243	PRO
1	C	301	PRO
1	D	301	PRO
1	A	255	GLU
1	A	445	LEU
1	B	240	LYS
1	B	241	ARG
1	C	229	TYR
1	D	300	ASN
1	A	246	ASN
1	A	359	GLN
1	B	185	ARG
1	B	246	ASN

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Mol	Chain	Res	Type
1	C	246	ASN
1	A	184	LYS
1	A	300	ASN
1	A	358	PHE
1	C	244	ARG
1	D	244	ARG

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	332/338 (98%)	318 (96%)	14 (4%)	30	54
1	B	332/338 (98%)	322 (97%)	10 (3%)	41	68
1	C	332/338 (98%)	322 (97%)	10 (3%)	41	68
1	D	332/338 (98%)	323 (97%)	9 (3%)	44	71
All	All	1328/1352 (98%)	1285 (97%)	43 (3%)	39	65

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	GLU
1	A	195	LEU
1	A	231	THR
1	A	242	ILE
1	A	354	ASP
1	A	396	GLU
1	A	423	VAL
1	A	443	ARG
1	A	453	LEU
1	A	461	ARG
1	A	475	LEU
1	A	483	ARG
1	A	498	ASN
1	A	507	LEU
1	B	192	VAL

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Mol	Chain	Res	Type
1	B	195	LEU
1	B	236	LEU
1	B	262	MET
1	B	299	ARG
1	B	329	GLN
1	B	380	ILE
1	B	430	MET
1	B	503	ILE
1	B	507	LEU
1	C	176	GLU
1	C	188	GLU
1	C	195	LEU
1	C	225	LEU
1	C	229	TYR
1	C	246	ASN
1	C	277	ILE
1	C	301	PRO
1	C	457	LEU
1	C	507	LEU
1	D	160	LYS
1	D	161	ARG
1	D	195	LEU
1	D	219	GLU
1	D	256	VAL
1	D	300	ASN
1	D	303	GLU
1	D	320	ILE
1	D	354	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	356	ASN
1	A	359	GLN
1	B	300	ASN
1	B	359	GLN
1	C	300	ASN
1	C	359	GLN
1	C	377	ASN
1	C	444	ASN
1	C	499	ASN

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Mol	Chain	Res	Type
1	D	499	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	359/366 (98%)	-0.37	6 (1%) 70 72	26, 45, 82, 127	0
1	B	359/366 (98%)	-0.47	4 (1%) 80 82	23, 39, 70, 128	0
1	C	359/366 (98%)	-0.50	5 (1%) 75 77	25, 40, 70, 133	0
1	D	359/366 (98%)	-0.48	4 (1%) 80 82	21, 42, 67, 133	0
2	E	18/18 (100%)	-0.85	0 100 100	25, 41, 89, 105	0
2	F	18/18 (100%)	-0.67	0 100 100	29, 49, 107, 109	0
2	G	18/18 (100%)	-0.93	0 100 100	28, 42, 84, 93	0
2	H	18/18 (100%)	-0.76	0 100 100	33, 48, 96, 97	0
2	I	18/18 (100%)	-0.61	0 100 100	37, 85, 115, 133	0
2	J	18/18 (100%)	-0.74	0 100 100	36, 61, 100, 112	0
2	K	18/18 (100%)	-0.94	0 100 100	29, 47, 72, 73	0
2	L	18/18 (100%)	-0.85	0 100 100	32, 44, 76, 86	0
All	All	1580/1608 (98%)	-0.49	19 (1%) 79 80	21, 42, 80, 133	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	PRO	7.5
1	B	507	LEU	6.1
1	A	241	ARG	5.5
1	D	243	PRO	5.4
1	A	242	ILE	4.9
1	A	244	ARG	4.8
1	A	254	GLY	4.0
1	D	245	GLY	3.9
1	B	245	GLY	3.8
1	C	241	ARG	3.8
1	D	244	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	244	ARG	3.6
1	C	243	PRO	3.2
1	D	241	ARG	2.8
1	B	241	ARG	2.7
1	C	244	ARG	2.4
1	C	245	GLY	2.1
1	C	242	ILE	2.1
1	A	229	TYR	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. 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(\AA^2)	Q<0.9
3	ZN	A	601	1/1	0.99	0.14	45,45,45,45	0
3	ZN	D	601	1/1	0.99	0.14	46,46,46,46	0
3	ZN	B	601	1/1	1.00	0.15	43,43,43,43	0
3	ZN	C	601	1/1	1.00	0.14	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.