



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:09 am BST

PDB ID : 3ZC0
Title : Structure of AfC3PO - duplex RNA complex
Authors : Parizotto, E.A.; Lowe, E.D.; Parker, J.S.
Deposited on : 2012-11-14
Resolution : 2.98 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

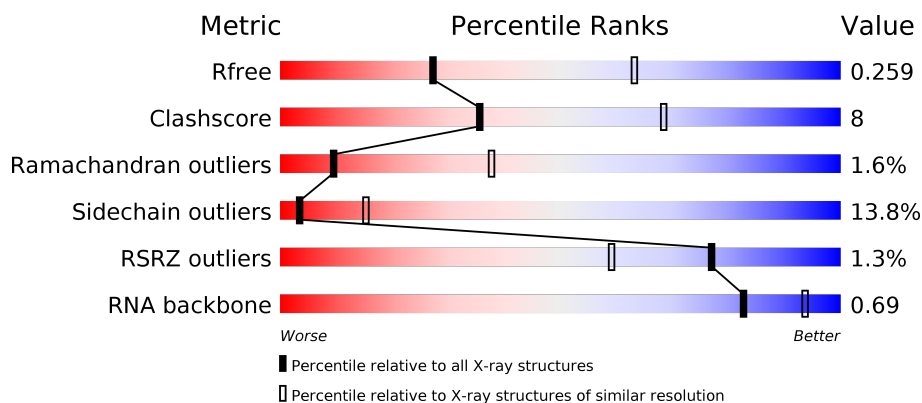
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)
RNA backbone	3102	1088 (3.26-2.70)

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	199	<div> <div>2%</div> <div>65% 25% 6% • 5%</div> </div>
1	B	199	<div> <div>0%</div> <div>69% 23% • •</div> </div>
1	C	199	<div> <div>2%</div> <div>72% 18% 5% 5%</div> </div>
1	D	199	<div> <div>0%</div> <div>72% 17% 5% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain			
1	E	199	<div><div><div>4%</div><div></div></div><div><div></div><div>66%</div></div><div><div></div><div>25%</div></div><div><div></div><div>5%</div></div></div>			
1	F	199	<div><div><div>%</div><div></div></div><div><div></div><div>69%</div></div><div><div></div><div>23%</div></div><div><div></div><div>5%</div></div></div>			
1	G	199	<div><div><div></div><div>69%</div></div><div><div></div><div>20%</div></div><div><div></div><div>6%</div></div><div><div></div><div>5%</div></div></div>			
1	H	199	<div><div><div>%</div><div></div></div><div><div></div><div>70%</div></div><div><div></div><div>20%</div></div><div><div></div><div>6%</div></div></div>			
1	I	199	<div><div><div>5%</div><div></div></div><div><div></div><div>68%</div></div><div><div></div><div>23%</div></div><div><div></div><div>5%</div></div></div>			
1	J	199	<div><div><div>%</div><div></div></div><div><div></div><div>70%</div></div><div><div></div><div>22%</div></div><div><div></div><div>5%</div></div></div>			
1	K	199	<div><div><div></div><div>70%</div></div><div><div></div><div>20%</div></div><div><div></div><div>5%</div></div><div><div></div><div>5%</div></div></div>			
1	L	199	<div><div><div>%</div><div></div></div><div><div></div><div>69%</div></div><div><div></div><div>21%</div></div><div><div></div><div>6%</div></div></div>			
2	M	16	<div><div><div></div><div>69%</div></div><div><div></div><div>25%</div></div><div><div></div><div>6%</div></div></div>			
2	N	16	<div><div><div>6%</div><div></div></div><div><div></div><div>69%</div></div><div><div></div><div>25%</div></div><div><div></div><div>6%</div></div></div>			
2	O	16	<div><div><div>13%</div><div></div></div><div><div></div><div>56%</div></div><div><div></div><div>38%</div></div><div><div></div><div>6%</div></div></div>			

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19888 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 AFTRAX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1517	969	255	285	8			
1	B	191	Total	C	N	O	S	0	0	0
			1531	977	261	285	8			
1	C	189	Total	C	N	O	S	0	1	0
			1510	964	253	285	8			
1	D	187	Total	C	N	O	S	0	1	0
			1492	953	251	280	8			
1	E	190	Total	C	N	O	S	0	0	0
			1505	961	253	283	8			
1	F	190	Total	C	N	O	S	0	0	0
			1520	971	259	283	7			
1	G	189	Total	C	N	O	S	0	0	0
			1500	958	252	282	8			
1	H	187	Total	C	N	O	S	0	1	0
			1485	949	250	278	8			
1	I	190	Total	C	N	O	S	0	0	0
			1506	963	254	281	8			
1	J	190	Total	C	N	O	S	0	2	0
			1534	976	262	288	8			
1	K	189	Total	C	N	O	S	0	0	0
			1502	959	255	280	8			
1	L	187	Total	C	N	O	S	0	2	0
			1504	960	255	281	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O28024
A	-1	PRO	-	expression tag	UNP O28024
A	0	HIS	-	expression tag	UNP O28024
A	114	ALA	ASP	engineered mutation	UNP O28024
B	-2	GLY	-	expression tag	UNP O28024

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	PRO	-	expression tag	UNP O28024
B	0	HIS	-	expression tag	UNP O28024
B	114	ALA	ASP	engineered mutation	UNP O28024
C	-2	GLY	-	expression tag	UNP O28024
C	-1	PRO	-	expression tag	UNP O28024
C	0	HIS	-	expression tag	UNP O28024
C	114	ALA	ASP	engineered mutation	UNP O28024
D	-2	GLY	-	expression tag	UNP O28024
D	-1	PRO	-	expression tag	UNP O28024
D	0	HIS	-	expression tag	UNP O28024
D	114	ALA	ASP	engineered mutation	UNP O28024
E	-2	GLY	-	expression tag	UNP O28024
E	-1	PRO	-	expression tag	UNP O28024
E	0	HIS	-	expression tag	UNP O28024
E	114	ALA	ASP	engineered mutation	UNP O28024
F	-2	GLY	-	expression tag	UNP O28024
F	-1	PRO	-	expression tag	UNP O28024
F	0	HIS	-	expression tag	UNP O28024
F	114	ALA	ASP	engineered mutation	UNP O28024
G	-2	GLY	-	expression tag	UNP O28024
G	-1	PRO	-	expression tag	UNP O28024
G	0	HIS	-	expression tag	UNP O28024
G	114	ALA	ASP	engineered mutation	UNP O28024
H	-2	GLY	-	expression tag	UNP O28024
H	-1	PRO	-	expression tag	UNP O28024
H	0	HIS	-	expression tag	UNP O28024
H	114	ALA	ASP	engineered mutation	UNP O28024
I	-2	GLY	-	expression tag	UNP O28024
I	-1	PRO	-	expression tag	UNP O28024
I	0	HIS	-	expression tag	UNP O28024
I	114	ALA	ASP	engineered mutation	UNP O28024
J	-2	GLY	-	expression tag	UNP O28024
J	-1	PRO	-	expression tag	UNP O28024
J	0	HIS	-	expression tag	UNP O28024
J	114	ALA	ASP	engineered mutation	UNP O28024
K	-2	GLY	-	expression tag	UNP O28024
K	-1	PRO	-	expression tag	UNP O28024
K	0	HIS	-	expression tag	UNP O28024
K	114	ALA	ASP	engineered mutation	UNP O28024
L	-2	GLY	-	expression tag	UNP O28024
L	-1	PRO	-	expression tag	UNP O28024
L	0	HIS	-	expression tag	UNP O28024

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Chain	Residue	Modelled	Actual	Comment	Reference
L	114	ALA	ASP	engineered mutation	UNP O28024

- Molecule 2 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*GP*CP*GP*UP*CP*GP*AP*AP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	15	Total	C	N	O	P	0	15	0
			560	247	99	186	28			
2	N	15	Total	C	N	O	P	0	15	0
			560	247	99	186	28			
2	O	15	Total	C	N	O	P	0	15	0
			560	247	99	186	28			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	L	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

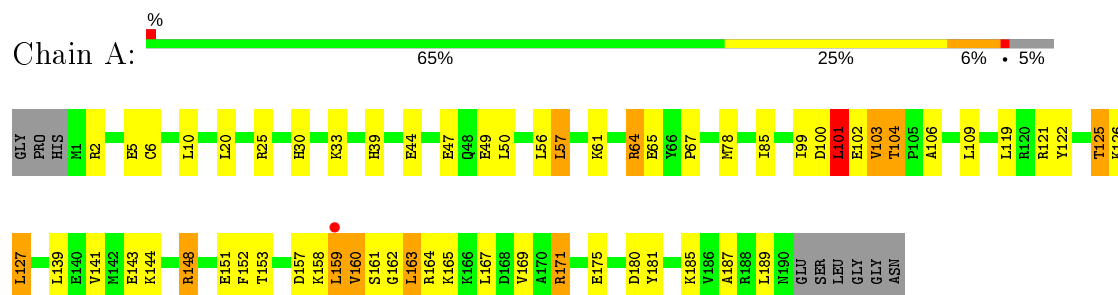
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	8	Total O 8 8	0	0
5	C	12	Total O 12 12	0	0
5	D	3	Total O 3 3	0	0
5	E	4	Total O 4 4	0	0
5	F	11	Total O 11 11	0	0
5	G	14	Total O 14 14	0	0
5	H	3	Total O 3 3	0	0
5	I	3	Total O 3 3	0	0
5	J	7	Total O 7 7	0	0
5	K	13	Total O 13 13	0	0
5	L	4	Total O 4 4	0	0

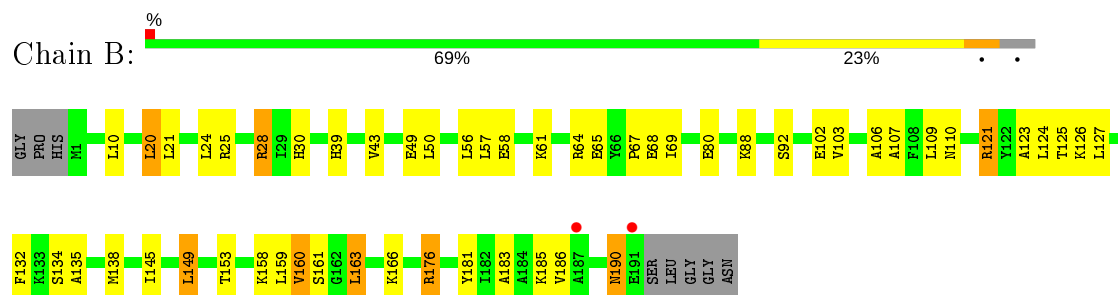
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

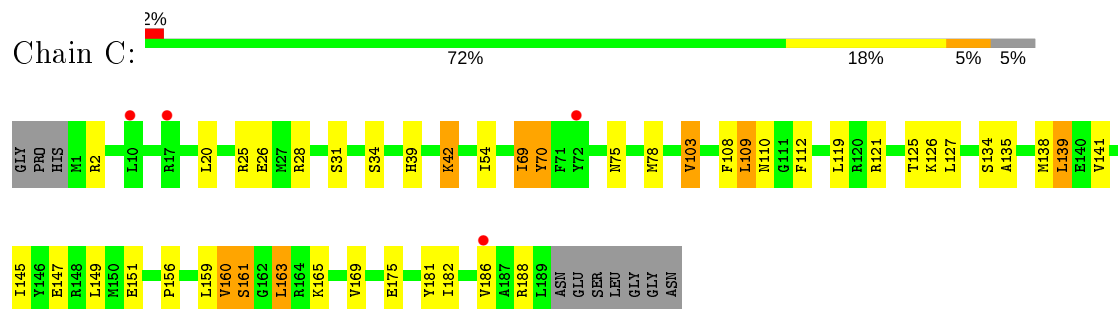
• Molecule 1: AFTRAX



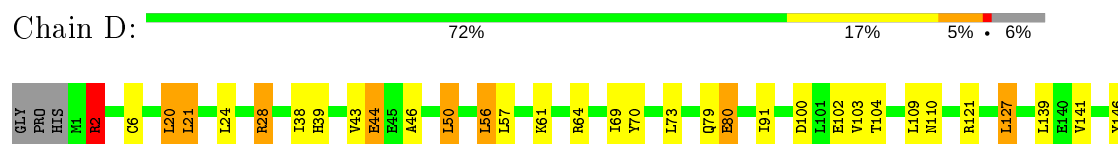
• Molecule 1: AFTRAX



• Molecule 1: AFTRAX



• Molecule 1: AFTRAX

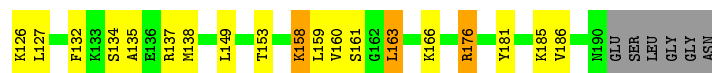




- Molecule 1: AFTRAX



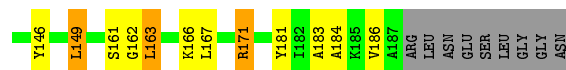
- Molecule 1: AFTRAX



- Molecule 1: AFTRAX



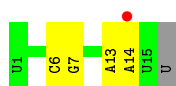
- Molecule 1: AFTRAX



- Molecule 1: AFTRAX







● Molecule 2: 5'-R(*UP*UP*CP*GP*AP*CP*GP*CP*GP*UP*CP*GP*AP*AP*UP*U)-3',



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.06 Å 183.06 Å 198.12 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.09 – 2.98 123.78 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (83.09-2.98) 100.0 (123.78-2.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.96 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.257 0.212 , 0.259	Depositor DCC
R_{free} test set	3949 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19888	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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 33.51 % 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 7.9016e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/1537	0.65	1/2062 (0.0%)
1	B	0.49	0/1551	0.65	0/2079
1	C	0.51	0/1533	0.63	0/2059
1	D	0.50	1/1512 (0.1%)	0.61	0/2030
1	E	0.50	0/1525	0.65	1/2049 (0.0%)
1	F	0.50	0/1540	0.64	0/2065
1	G	0.51	0/1520	0.64	0/2042
1	H	0.48	0/1505	0.61	0/2022
1	I	0.51	0/1526	0.66	1/2049 (0.0%)
1	J	0.52	0/1554	0.67	0/2086
1	K	0.50	0/1522	0.63	0/2044
1	L	0.49	0/1524	0.60	0/2045
2	M	14.01	2/646 (0.3%)	2.71	8/1003 (0.8%)
2	N	13.99	2/646 (0.3%)	2.69	8/1003 (0.8%)
2	O	0.42	0/645	0.94	0/999
All	All	3.57	5/20286 (0.0%)	0.96	19/27637 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	14[A]	A	P-O5'	251.74	4.11	1.59
2	M	14[B]	A	P-O5'	251.74	4.11	1.59
2	N	14[A]	A	P-O5'	251.36	4.11	1.59
2	N	14[B]	A	P-O5'	251.36	4.11	1.59
1	D	6	CYS	CB-SG	-5.00	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	14[A]	A	O5'-P-OP2	39.06	157.57	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	14[B]	A	O5'-P-OP2	39.06	157.57	110.70
2	N	14[A]	A	O5'-P-OP2	38.74	157.19	110.70
2	N	14[B]	A	O5'-P-OP2	38.74	157.19	110.70
2	M	14[A]	A	P-O5'-C5'	-29.34	73.96	120.90
2	M	14[B]	A	P-O5'-C5'	-29.34	73.96	120.90
2	N	14[A]	A	P-O5'-C5'	-29.14	74.28	120.90
2	N	14[B]	A	P-O5'-C5'	-29.14	74.28	120.90
2	M	14[A]	A	O5'-P-OP1	-24.29	81.56	110.70
2	M	14[B]	A	O5'-P-OP1	-24.29	81.56	110.70
2	N	14[A]	A	O5'-P-OP1	-23.91	82.01	110.70
2	N	14[B]	A	O5'-P-OP1	-23.91	82.01	110.70
2	N	13[A]	A	O3'-P-O5'	-20.25	65.52	104.00
2	N	13[B]	A	O3'-P-O5'	-20.25	65.52	104.00
2	M	13[A]	A	O3'-P-O5'	-20.23	65.57	104.00
2	M	13[B]	A	O3'-P-O5'	-20.23	65.57	104.00
1	E	101	LEU	CA-CB-CG	5.61	128.20	115.30
1	I	101	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	101	LEU	CA-CB-CG	5.48	127.91	115.30

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	1517	0	1539	37	0
1	B	1531	0	1563	27	0
1	C	1510	0	1523	24	0
1	D	1492	0	1504	21	0
1	E	1505	0	1513	30	0
1	F	1520	0	1550	24	0
1	G	1500	0	1511	28	0
1	H	1485	0	1491	24	0
1	I	1506	0	1522	26	0
1	J	1534	0	1545	26	0
1	K	1502	0	1518	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1504	0	1518	24	0
2	M	560	0	281	1	0
2	N	560	0	281	1	0
2	O	560	0	281	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	B	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	K	1	0	0	0	0
5	A	4	0	0	0	0
5	B	8	0	0	0	0
5	C	12	0	0	1	0
5	D	3	0	0	0	0
5	E	4	0	0	0	0
5	F	11	0	0	1	0
5	G	14	0	0	2	0
5	H	3	0	0	0	0
5	I	3	0	0	0	0
5	J	7	0	0	0	0
5	K	13	0	0	2	0
5	L	4	0	0	0	0
All	All	19888	0	19140	317	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 8.

All (317) 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:158:LYS:H	1:A:161:SER:H	1.21	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLU:HA	1:E:103:VAL:HB	1.59	0.82
1:I:102:GLU:HA	1:I:103:VAL:HB	1.61	0.82
1:A:102:GLU:HA	1:A:103:VAL:HB	1.60	0.81
1:K:69:ILE:HG13	1:K:70:TYR:H	1.50	0.77
1:K:39:HIS:CE1	1:K:121:ARG:HG2	2.20	0.76
1:C:69:ILE:HG13	1:C:70:TYR:H	1.51	0.75
1:C:39:HIS:CE1	1:C:121:ARG:HG2	2.22	0.74
1:E:157:ASP:O	1:E:159:LEU:N	2.20	0.74
1:A:148:ARG:NH2	1:A:151:GLU:OE1	2.20	0.73
1:J:39:HIS:CE1	1:J:121:ARG:HG2	2.24	0.73
1:B:39:HIS:CE1	1:B:121:ARG:HG2	2.24	0.72
1:F:39:HIS:CE1	1:F:121:ARG:HG2	2.24	0.72
1:G:39:HIS:CE1	1:G:121:ARG:HG2	2.23	0.72
1:G:69:ILE:HG13	1:G:70:TYR:H	1.55	0.72
1:G:45:GLU:HA	1:G:48:GLN:HG2	1.71	0.71
1:E:160:VAL:HG13	1:E:163:LEU:HB2	1.73	0.70
1:J:30:HIS:ND1	1:J:49:GLU:OE1	2.26	0.67
1:I:30:HIS:ND1	1:I:49:GLU:OE1	2.27	0.66
1:E:30:HIS:ND1	1:E:49:GLU:OE1	2.29	0.66
1:A:160:VAL:HG13	1:A:163:LEU:HB2	1.77	0.65
1:F:30:HIS:ND1	1:F:49:GLU:OE1	2.27	0.64
1:D:28:ARG:NH1	1:D:80:GLU:OE2	2.31	0.63
1:F:28:ARG:HD2	1:F:80:GLU:HG3	1.80	0.63
1:H:39:HIS:CE1	1:H:121:ARG:HG2	2.34	0.63
1:B:28:ARG:HD2	1:B:80:GLU:HG3	1.81	0.63
1:A:30:HIS:ND1	1:A:49:GLU:OE1	2.33	0.62
1:B:30:HIS:ND1	1:B:49:GLU:OE1	2.28	0.61
1:L:39:HIS:CE1	1:L:121:ARG:HG2	2.36	0.61
1:I:157:ASP:O	1:I:159:LEU:N	2.33	0.61
1:D:39:HIS:CE1	1:D:121:ARG:HG2	2.37	0.60
1:E:157:ASP:N	1:E:157:ASP:OD1	2.26	0.59
1:A:158:LYS:N	1:A:161:SER:H	1.96	0.59
1:D:28:ARG:CZ	1:D:80:GLU:HG3	2.33	0.59
1:K:45:GLU:HA	1:K:48:GLN:HG2	1.85	0.59
1:L:146:TYR:CZ	1:L:171:ARG:HG2	2.40	0.57
1:A:158:LYS:H	1:A:161:SER:N	1.99	0.57
1:D:146:TYR:CZ	1:D:171:ARG:HG2	2.39	0.57
1:L:153:THR:HG23	1:L:164:ARG:HD2	1.86	0.57
1:L:21:LEU:HD21	1:L:73:LEU:HD22	1.87	0.57
1:D:38:ILE:HD13	1:D:91:ILE:HG12	1.88	0.56
1:H:183:ALA:HA	1:H:186:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ALA:HA	1:D:186:VAL:HG12	1.88	0.56
1:H:38:ILE:HD13	1:H:91:ILE:HG12	1.88	0.56
1:H:161:SER:OG	1:H:162:GLY:N	2.39	0.55
1:L:183:ALA:HA	1:L:186:VAL:HG12	1.88	0.55
1:G:137:ARG:HD3	1:J:137:ARG:HE	1.71	0.55
1:L:161:SER:OG	1:L:162:GLY:N	2.38	0.55
1:G:69:ILE:HG13	1:G:70:TYR:N	2.23	0.54
1:C:69:ILE:HG13	1:C:70:TYR:N	2.22	0.54
1:H:146:TYR:CZ	1:H:171:ARG:HG2	2.42	0.54
1:K:69:ILE:HG13	1:K:70:TYR:N	2.19	0.54
1:K:121:ARG:O	1:K:125:THR:HG23	2.08	0.53
1:A:158:LYS:CA	1:A:160:VAL:H	2.20	0.53
1:H:21:LEU:HD21	1:H:73:LEU:HD22	1.90	0.53
1:I:160:VAL:HG13	1:I:163:LEU:HB2	1.89	0.53
1:C:78:MET:HB3	1:C:103:VAL:HG22	1.90	0.53
1:F:106:ALA:O	1:F:110:ASN:HB2	2.08	0.53
1:B:64:ARG:NH1	1:B:102:GLU:OE1	2.42	0.53
1:J:64:ARG:NH1	1:J:102:GLU:OE1	2.42	0.52
1:J:106:ALA:O	1:J:110:ASN:HB2	2.09	0.52
1:D:161:SER:OG	1:D:162:GLY:N	2.42	0.52
1:I:121:ARG:O	1:I:125:THR:HG22	2.08	0.52
1:A:106:ALA:HB2	1:A:159:LEU:O	2.08	0.52
1:E:121:ARG:O	1:E:125:THR:HG22	2.09	0.52
1:A:121:ARG:O	1:A:125:THR:HG22	2.10	0.52
1:K:153:THR:HG23	1:K:164:ARG:HD3	1.92	0.52
1:J:132:PHE:HE2	1:J:185:LYS:HA	1.75	0.51
1:B:134:SER:O	1:B:138:MET:HG2	2.10	0.51
1:H:57:LEU:HD11	1:H:61:LYS:HE2	1.91	0.51
1:I:143:GLU:OE1	1:I:171:ARG:NH2	2.42	0.51
1:F:132:PHE:HE2	1:F:185:LYS:HA	1.74	0.51
1:G:78:MET:HB3	1:G:103:VAL:HG22	1.92	0.51
1:G:121:ARG:O	1:G:125:THR:HG23	2.10	0.51
1:D:110:ASN:OD1	1:D:166:LYS:HD3	2.12	0.50
1:F:88:LYS:NZ	1:F:92:SER:OG	2.38	0.50
1:F:64:ARG:NH1	1:F:102:GLU:OE1	2.43	0.50
1:F:134:SER:O	1:F:138:MET:HG2	2.11	0.50
1:L:38:ILE:HD13	1:L:91:ILE:HG12	1.94	0.50
1:B:132:PHE:HE2	1:B:185:LYS:HA	1.75	0.50
1:A:143:GLU:OE1	1:A:171:ARG:NH2	2.44	0.50
1:D:28:ARG:NH2	1:D:80:GLU:HG3	2.26	0.50
1:K:145:ILE:O	1:K:149:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LEU:HD21	1:D:73:LEU:HD22	1.94	0.50
1:J:103:VAL:HG13	1:J:107:ALA:HB3	1.93	0.50
1:A:99:ILE:O	1:A:99:ILE:HG13	2.12	0.49
1:I:153:THR:O	1:I:164:ARG:NH2	2.45	0.49
1:E:143:GLU:OE1	1:E:171:ARG:NH2	2.45	0.49
1:E:78:MET:HE3	1:E:104:THR:HG22	1.94	0.49
1:F:103:VAL:HG13	1:F:107:ALA:HB3	1.94	0.49
1:J:134:SER:O	1:J:138:MET:HG2	2.12	0.49
1:A:153:THR:O	1:A:164:ARG:NH2	2.46	0.49
1:E:78:MET:HB3	1:E:103:VAL:HG22	1.95	0.49
1:G:127:LEU:HD12	1:G:127:LEU:HA	1.65	0.49
1:C:121:ARG:O	1:C:125:THR:HG23	2.13	0.49
1:K:25:ARG:NH1	5:K:2001:HOH:O	2.45	0.49
1:A:78:MET:HE3	1:A:104:THR:HG22	1.95	0.48
1:H:110:ASN:OD1	1:H:166:LYS:HD3	2.12	0.48
1:B:103:VAL:HG13	1:B:107:ALA:HB3	1.95	0.48
1:B:110:ASN:OD1	1:B:166:LYS:HD3	2.14	0.48
1:K:127:LEU:HD21	1:K:181:TYR:HA	1.94	0.48
1:B:127:LEU:HD13	1:B:135:ALA:CB	2.43	0.48
1:C:127:LEU:HD21	1:C:181:TYR:HA	1.96	0.48
1:I:122:TYR:CZ	1:I:126:LYS:HE2	2.48	0.48
1:G:145:ILE:O	1:G:149:LEU:HB2	2.13	0.48
1:B:106:ALA:O	1:B:110:ASN:HB2	2.14	0.48
1:C:145:ILE:O	1:C:149:LEU:HB2	2.13	0.48
1:E:99:ILE:HG13	1:E:99:ILE:O	2.13	0.48
1:I:3:LEU:HD23	1:I:3:LEU:HA	1.73	0.48
1:I:78:MET:HE3	1:I:104:THR:HG22	1.96	0.48
2:O:6[B]:C:H2'	2:O:7[B]:G:C8	2.49	0.48
1:B:88:LYS:NZ	1:B:92:SER:OG	2.40	0.47
1:J:110:ASN:OD1	1:J:166:LYS:HD3	2.14	0.47
1:L:110:ASN:OD1	1:L:166:LYS:HD3	2.13	0.47
1:L:157:ASP:H	1:L:164:ARG:HH21	1.59	0.47
1:G:139:LEU:HA	1:G:139:LEU:HD12	1.72	0.47
1:I:44:GLU:O	1:I:47:GLU:HB3	2.14	0.47
1:C:121:ARG:NH1	5:C:2009:HOH:O	2.29	0.47
1:D:146:TYR:CE1	1:D:171:ARG:HG2	2.48	0.47
1:D:2:ARG:HD2	1:D:2:ARG:HA	1.64	0.47
1:E:161:SER:OG	1:E:162:GLY:N	2.45	0.47
1:E:39:HIS:CE1	1:E:121:ARG:HB2	2.50	0.47
1:I:65:GLU:O	1:I:67:PRO:HD3	2.15	0.47
1:A:44:GLU:O	1:A:47:GLU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:TYR:CZ	1:E:126:LYS:HE2	2.49	0.47
1:A:163:LEU:HD22	1:A:167:LEU:HG	1.96	0.47
1:K:110:ASN:ND2	1:K:161:SER:HB3	2.30	0.47
1:A:161:SER:OG	1:A:162:GLY:N	2.47	0.47
1:I:78:MET:HB3	1:I:103:VAL:HG22	1.96	0.47
1:C:110:ASN:ND2	1:C:161:SER:HB3	2.31	0.46
1:J:88:LYS:NZ	1:J:92:SER:OG	2.41	0.46
1:F:158:LYS:NZ	5:F:2011:HOH:O	2.43	0.46
1:K:78:MET:HB3	1:K:103:VAL:HG22	1.96	0.46
1:G:25:ARG:NH1	5:G:2001:HOH:O	2.48	0.46
1:A:122:TYR:CZ	1:A:126:LYS:HE2	2.51	0.46
1:A:78:MET:HB3	1:A:103:VAL:HG22	1.98	0.46
1:B:132:PHE:CE2	1:B:185:LYS:HA	2.51	0.46
1:C:182:ILE:O	1:C:186:VAL:HG12	2.16	0.46
1:F:127:LEU:HD13	1:F:135:ALA:CB	2.45	0.46
1:I:85:ILE:HD13	1:I:101:LEU:HD11	1.98	0.46
1:K:160:VAL:O	1:K:163:LEU:HB2	2.15	0.46
1:B:183:ALA:HB1	1:C:186:VAL:HG11	1.97	0.46
1:L:97:PHE:CE2	1:L:148:ARG:HG2	2.51	0.46
1:A:85:ILE:HD13	1:A:101:LEU:HD11	1.99	0.45
1:I:163:LEU:HD22	1:I:167:LEU:HG	1.97	0.45
1:K:156:PRO:HG2	1:K:159:LEU:HD12	1.97	0.45
1:J:183:ALA:HB1	1:K:186:VAL:HG11	1.98	0.45
1:J:132:PHE:CE2	1:J:185:LYS:HA	2.51	0.45
1:K:182:ILE:O	1:K:186:VAL:HG12	2.17	0.45
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.74	0.45
1:F:110:ASN:OD1	1:F:166:LYS:HD3	2.16	0.45
1:I:99:ILE:HG13	1:I:99:ILE:O	2.15	0.45
1:J:144:LYS:HG3	1:J:148:ARG:NH2	2.31	0.45
1:F:20:LEU:HD22	1:F:24:LEU:HG	1.99	0.45
1:H:149:LEU:HD12	1:H:149:LEU:HA	1.77	0.45
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.68	0.45
1:G:144:LYS:HE3	1:G:144:LYS:HB2	1.78	0.45
1:J:127:LEU:HD13	1:J:135:ALA:CB	2.46	0.45
1:F:132:PHE:CE2	1:F:185:LYS:HA	2.50	0.45
1:G:121:ARG:NH1	5:G:2010:HOH:O	2.28	0.45
1:I:126:LYS:HA	1:I:126:LYS:HD3	1.78	0.45
1:I:161:SER:OG	1:I:162:GLY:N	2.50	0.45
1:I:185:LYS:HD2	1:I:185:LYS:HA	1.65	0.45
1:E:163:LEU:HD22	1:E:167:LEU:HG	1.99	0.45
1:E:57:LEU:HD13	1:E:61:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:LYS:H	1:K:42:LYS:HG2	1.39	0.44
1:E:44:GLU:O	1:E:47:GLU:HB3	2.17	0.44
1:G:110:ASN:ND2	1:G:161:SER:HB3	2.32	0.44
1:G:182:ILE:O	1:G:186:VAL:HG12	2.16	0.44
1:H:19:GLU:HB3	1:H:63:TYR:OH	2.17	0.44
1:I:57:LEU:HD13	1:I:61:LYS:HE2	1.99	0.44
1:L:157:ASP:N	1:L:164:ARG:HH21	2.16	0.44
1:A:57:LEU:HD13	1:A:61:LYS:HE2	1.99	0.44
1:C:127:LEU:HA	1:C:127:LEU:HD12	1.65	0.44
1:D:57:LEU:HD11	1:D:61:LYS:HE2	2.00	0.44
1:F:126:LYS:HD3	1:F:126:LYS:HA	1.80	0.44
1:H:127:LEU:HD21	1:H:181:TYR:HA	2.00	0.44
1:I:102:GLU:HB3	1:I:103:VAL:O	2.17	0.44
1:A:158:LYS:HD3	1:A:161:SER:HB3	1.99	0.44
1:B:20:LEU:HD22	1:B:24:LEU:HG	2.00	0.44
1:E:127:LEU:HD21	1:E:181:TYR:HA	2.00	0.44
1:E:3:LEU:HA	1:E:3:LEU:HD23	1.83	0.44
1:B:58:GLU:OE1	1:B:61:LYS:NZ	2.47	0.44
1:G:119:LEU:HA	1:G:119:LEU:HD23	1.82	0.44
1:G:21:LEU:HD21	1:G:73:LEU:HD12	2.00	0.44
1:A:126:LYS:HA	1:A:126:LYS:HD3	1.78	0.44
1:A:158:LYS:HD2	1:A:158:LYS:HA	1.88	0.44
1:A:165:LYS:O	1:A:169:VAL:HG23	2.18	0.44
1:E:10:LEU:HD12	1:E:10:LEU:HA	1.91	0.44
1:L:127:LEU:HD21	1:L:181:TYR:HA	2.00	0.44
1:C:109:LEU:HD12	1:C:109:LEU:HA	1.88	0.44
1:F:159:LEU:HA	1:F:159:LEU:HD23	1.73	0.44
1:J:126:LYS:HA	1:J:126:LYS:HD3	1.83	0.44
1:K:116:VAL:HG11	1:K:170:ALA:HB1	1.98	0.44
1:L:146:TYR:CE1	1:L:171:ARG:HG2	2.54	0.43
1:H:2:ARG:HD2	1:H:2:ARG:HA	1.59	0.43
1:J:123:ALA:O	1:J:127:LEU:HB2	2.18	0.43
1:K:45:GLU:HA	1:K:48:GLN:CG	2.48	0.43
1:A:102:GLU:HB3	1:A:103:VAL:O	2.19	0.43
1:E:102:GLU:HB3	1:E:103:VAL:O	2.18	0.43
1:G:127:LEU:HD21	1:G:181:TYR:HA	1.99	0.43
1:K:139:LEU:HD12	1:K:139:LEU:HA	1.79	0.43
1:C:119:LEU:HA	1:C:119:LEU:HD23	1.80	0.43
1:H:127:LEU:HA	1:H:127:LEU:HD12	1.81	0.43
1:L:33:LYS:HD2	1:L:33:LYS:HA	1.64	0.43
1:L:3:LEU:HA	1:L:3:LEU:HD23	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD21	1:A:181:TYR:HA	2.00	0.43
1:C:42:LYS:H	1:C:42:LYS:HG2	1.35	0.43
1:L:167:LEU:HD23	1:L:167:LEU:HA	1.91	0.43
1:F:127:LEU:HD21	1:F:181:TYR:HA	2.01	0.43
1:H:183:ALA:O	1:H:184:ALA:HB3	2.18	0.43
1:J:190:ASN:N	1:J:190:ASN:OD1	2.52	0.43
1:J:21:LEU:HD23	1:J:21:LEU:HA	1.87	0.43
1:G:108:PHE:CZ	1:G:112:PHE:HE2	2.37	0.43
1:I:182:ILE:HG23	1:L:184:ALA:HB2	1.99	0.43
1:C:156:PRO:HG2	1:C:159:LEU:HD12	2.00	0.43
1:H:79:GLN:HG3	1:H:80:GLU:N	2.34	0.43
1:K:108:PHE:CZ	1:K:112:PHE:HE2	2.37	0.43
1:K:126:LYS:HD3	1:K:134:SER:HB2	1.99	0.43
1:L:183:ALA:O	1:L:184:ALA:HB3	2.19	0.43
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.87	0.43
1:F:123:ALA:O	1:F:127:LEU:HB2	2.19	0.43
1:L:44:GLU:CD	1:L:44:GLU:H	2.23	0.43
1:B:126:LYS:HD3	1:B:126:LYS:HA	1.82	0.42
1:H:146:TYR:CE1	1:H:171:ARG:HG2	2.54	0.42
1:A:64:ARG:HE	1:A:64:ARG:HB3	1.62	0.42
1:E:119:LEU:HD23	1:E:119:LEU:HA	1.92	0.42
1:H:167:LEU:HA	1:H:167:LEU:HD23	1.91	0.42
1:I:127:LEU:HD21	1:I:181:TYR:HA	2.00	0.42
1:I:94:GLU:H	1:I:94:GLU:HG2	1.68	0.42
1:J:148:ARG:HD3	1:J:148:ARG:HA	1.65	0.42
1:B:127:LEU:HD21	1:B:181:TYR:HA	2.01	0.42
1:G:165:LYS:O	1:G:169:VAL:HG23	2.20	0.42
1:G:186:VAL:HG22	1:H:186:VAL:HG23	2.00	0.42
1:H:89:ASN:HB3	1:H:95:PHE:HA	2.02	0.42
2:N:6[B]:C:H2'	2:N:7[B]:G:C8	2.55	0.42
1:J:158:LYS:HE2	2:O:8[B]:C:OP2	2.19	0.42
1:G:156:PRO:HG2	1:G:159:LEU:HD12	2.01	0.42
1:A:109:LEU:HD21	1:A:152:PHE:CD2	2.55	0.42
1:C:126:LYS:HD3	1:C:134:SER:HB2	2.01	0.42
1:I:167:LEU:HA	1:I:167:LEU:HD23	1.85	0.42
1:L:149:LEU:HA	1:L:149:LEU:HD12	1.77	0.42
1:A:158:LYS:HD2	1:A:159:LEU:HA	2.01	0.42
1:A:185:LYS:C	1:A:187:ALA:H	2.23	0.42
1:B:123:ALA:O	1:B:127:LEU:HB2	2.20	0.42
1:D:20:LEU:HD22	1:D:24:LEU:HG	2.02	0.42
1:E:185:LYS:C	1:E:187:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:VAL:O	1:H:186:VAL:HG22	2.19	0.42
1:J:160:VAL:O	1:J:163:LEU:HB2	2.19	0.42
1:K:119:LEU:HA	1:K:119:LEU:HD23	1.82	0.42
1:E:185:LYS:HD2	1:E:185:LYS:HA	1.63	0.42
1:E:85:ILE:HD13	1:E:101:LEU:HD11	2.02	0.42
1:A:65:GLU:O	1:A:67:PRO:HD3	2.20	0.42
1:G:106:ALA:HB1	1:G:161:SER:HB2	2.02	0.42
1:J:20:LEU:HD22	1:J:24:LEU:HG	2.02	0.42
1:K:126:LYS:HD3	1:K:134:SER:CB	2.50	0.42
1:K:50:LEU:HA	1:K:50:LEU:HD23	1.75	0.42
1:A:185:LYS:HA	1:A:185:LYS:HD2	1.64	0.42
1:C:126:LYS:HD3	1:C:134:SER:CB	2.50	0.42
1:E:159:LEU:HA	1:E:159:LEU:HD23	1.85	0.42
1:E:96:THR:OG1	1:E:98:GLU:HG2	2.20	0.42
1:F:160:VAL:O	1:F:163:LEU:HB2	2.19	0.42
1:D:186:VAL:O	1:D:186:VAL:HG22	2.20	0.41
1:E:165:LYS:O	1:E:169:VAL:HG23	2.20	0.41
1:F:65:GLU:C	1:F:67:PRO:HD3	2.41	0.41
1:G:116:VAL:HG11	1:G:170:ALA:HB1	2.02	0.41
1:H:56:LEU:HD12	1:H:56:LEU:HA	1.77	0.41
1:L:43:VAL:O	1:L:46:ALA:HB3	2.20	0.41
1:A:180:ASP:HA	1:B:176:ARG:HH21	1.85	0.41
1:F:58:GLU:OE1	1:F:61:LYS:NZ	2.49	0.41
1:K:144:LYS:HE3	1:K:144:LYS:HB2	1.74	0.41
2:O:11[A]:C:H2'	2:O:12[A]:G:C8	2.56	0.41
1:B:160:VAL:O	1:B:163:LEU:HB2	2.21	0.41
1:C:139:LEU:HA	1:C:139:LEU:HD12	1.73	0.41
1:D:43:VAL:O	1:D:46:ALA:HB3	2.20	0.41
1:B:50:LEU:HD23	1:B:50:LEU:HA	1.77	0.41
1:A:39:HIS:CE1	1:A:121:ARG:HB2	2.55	0.41
1:E:180:ASP:HA	1:F:176:ARG:HH21	1.86	0.41
1:G:160:VAL:O	1:G:163:LEU:HB2	2.20	0.41
1:G:31:SER:O	1:G:34:SER:HB3	2.19	0.41
1:I:116:VAL:HG11	1:I:170:ALA:HB1	2.02	0.41
1:K:121:ARG:NH1	5:K:2009:HOH:O	2.25	0.41
1:K:159:LEU:HA	1:K:159:LEU:HD23	1.91	0.41
1:H:163:LEU:HA	1:H:163:LEU:HD23	1.91	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.92	0.41
1:C:108:PHE:CZ	1:C:112:PHE:HE2	2.39	0.41
1:C:165:LYS:O	1:C:169:VAL:HG23	2.20	0.41
1:G:44:GLU:OE2	1:G:45:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:186:VAL:O	1:L:186:VAL:HG22	2.21	0.41
1:B:145:ILE:O	1:B:149:LEU:HB2	2.21	0.41
1:F:124:LEU:HD12	1:F:124:LEU:HA	1.91	0.41
1:J:159:LEU:HD23	1:J:159:LEU:HA	1.66	0.41
1:L:100:ASP:O	1:L:101:LEU:HD23	2.21	0.41
1:F:50:LEU:HD23	1:F:50:LEU:HA	1.77	0.41
1:H:134:SER:O	1:H:138:MET:HG2	2.21	0.41
1:C:31:SER:O	1:C:34:SER:HB3	2.21	0.41
1:D:44:GLU:H	1:D:44:GLU:CD	2.24	0.41
1:D:50:LEU:HD23	1:D:50:LEU:HA	1.82	0.41
1:E:19:GLU:HB3	1:E:63:TYR:OH	2.21	0.41
1:K:25:ARG:O	1:K:29:ILE:HG13	2.21	0.41
1:B:124:LEU:HA	1:B:124:LEU:HD12	1.94	0.40
1:B:190:ASN:OD1	1:B:190:ASN:N	2.54	0.40
1:J:167:LEU:HD23	1:J:167:LEU:HA	1.92	0.40
1:K:27:MET:HE1	1:K:57:LEU:HD23	2.02	0.40
2:M:6[B]:C:H2'	2:M:7[B]:G:C8	2.56	0.40
1:B:65:GLU:C	1:B:67:PRO:HD3	2.42	0.40
1:C:160:VAL:O	1:C:163:LEU:HB2	2.21	0.40
1:D:127:LEU:HD21	1:D:181:TYR:HA	2.03	0.40
1:H:43:VAL:O	1:H:46:ALA:HB3	2.20	0.40
1:J:13:LEU:HA	1:J:13:LEU:HD23	1.84	0.40
1:L:85:ILE:HD13	1:L:101:LEU:HD11	2.03	0.40
1:J:158:LYS:HE2	2:O:9[A]:G:OP2	2.21	0.40
1:D:183:ALA:O	1:D:184:ALA:HB3	2.21	0.40
1:E:78:MET:CE	1:E:104:THR:HG22	2.51	0.40
1:C:127:LEU:HD13	1:C:135:ALA:CB	2.52	0.40
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.92	0.40
1:G:127:LEU:HD13	1:G:135:ALA:CB	2.52	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	188/199 (94%)	174 (93%)	12 (6%)	2 (1%)	14	47
1	B	189/199 (95%)	180 (95%)	7 (4%)	2 (1%)	14	47
1	C	188/199 (94%)	175 (93%)	11 (6%)	2 (1%)	14	47
1	D	186/199 (94%)	168 (90%)	13 (7%)	5 (3%)	5	24
1	E	188/199 (94%)	173 (92%)	11 (6%)	4 (2%)	7	30
1	F	188/199 (94%)	179 (95%)	8 (4%)	1 (0%)	29	66
1	G	187/199 (94%)	172 (92%)	13 (7%)	2 (1%)	14	47
1	H	186/199 (94%)	169 (91%)	12 (6%)	5 (3%)	5	24
1	I	188/199 (94%)	172 (92%)	12 (6%)	4 (2%)	7	30
1	J	190/199 (96%)	181 (95%)	7 (4%)	2 (1%)	14	47
1	K	187/199 (94%)	174 (93%)	11 (6%)	2 (1%)	14	47
1	L	187/199 (94%)	171 (91%)	11 (6%)	5 (3%)	5	24
All	All	2252/2388 (94%)	2088 (93%)	128 (6%)	36 (2%)	9	38

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	SER
1	D	2	ARG
1	F	161	SER
1	H	2	ARG
1	J	161	SER
1	L	2	ARG
1	A	103	VAL
1	C	70	TYR
1	D	70	TYR
1	D	102	GLU
1	E	103	VAL
1	E	157	ASP
1	E	158	LYS
1	G	70	TYR
1	H	70	TYR
1	H	102	GLU
1	I	103	VAL
1	I	157	ASP
1	K	70	TYR
1	L	70	TYR
1	L	102	GLU
1	C	69	ILE

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Mol	Chain	Res	Type
1	D	69	ILE
1	G	69	ILE
1	K	69	ILE
1	A	101	LEU
1	D	103	VAL
1	E	101	LEU
1	H	69	ILE
1	H	103	VAL
1	I	101	LEU
1	L	69	ILE
1	L	103	VAL
1	I	158	LYS
1	B	160	VAL
1	J	160	VAL

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	155/166 (93%)	128 (83%)	27 (17%)	2	9
1	B	157/166 (95%)	138 (88%)	19 (12%)	5	20
1	C	154/166 (93%)	134 (87%)	20 (13%)	4	17
1	D	151/166 (91%)	132 (87%)	19 (13%)	4	18
1	E	152/166 (92%)	126 (83%)	26 (17%)	2	9
1	F	155/166 (93%)	135 (87%)	20 (13%)	4	17
1	G	152/166 (92%)	131 (86%)	21 (14%)	3	15
1	H	149/166 (90%)	131 (88%)	18 (12%)	5	20
1	I	152/166 (92%)	129 (85%)	23 (15%)	3	12
1	J	156/166 (94%)	135 (86%)	21 (14%)	4	16
1	K	152/166 (92%)	132 (87%)	20 (13%)	4	16
1	L	152/166 (92%)	133 (88%)	19 (12%)	4	18
All	All	1837/1992 (92%)	1584 (86%)	253 (14%)	3	15

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	5	GLU
1	A	6	CYS
1	A	10	LEU
1	A	20	LEU
1	A	25	ARG
1	A	33	LYS
1	A	50	LEU
1	A	56	LEU
1	A	57	LEU
1	A	64	ARG
1	A	100	ASP
1	A	101	LEU
1	A	104	THR
1	A	125	THR
1	A	127	LEU
1	A	139	LEU
1	A	141	VAL
1	A	144	LYS
1	A	148	ARG
1	A	157	ASP
1	A	159	LEU
1	A	160	VAL
1	A	163	LEU
1	A	171	ARG
1	A	175	GLU
1	A	189	LEU
1	B	10	LEU
1	B	20	LEU
1	B	25	ARG
1	B	28	ARG
1	B	43	VAL
1	B	56	LEU
1	B	57	LEU
1	B	68	GLU
1	B	69	ILE
1	B	109	LEU
1	B	121	ARG
1	B	125	THR
1	B	149	LEU
1	B	153	THR
1	B	158	LYS

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Mol	Chain	Res	Type
1	B	163	LEU
1	B	176	ARG
1	B	186	VAL
1	B	190	ASN
1	C	2	ARG
1	C	20	LEU
1	C	25	ARG
1	C	26	GLU
1	C	28	ARG
1	C	42	LYS
1	C	54	ILE
1	C	75	ASN
1	C	103	VAL
1	C	109	LEU
1	C	138	MET
1	C	139	LEU
1	C	141	VAL
1	C	147	GLU
1	C	151	GLU
1	C	160	VAL
1	C	161	SER
1	C	163	LEU
1	C	175	GLU
1	C	188	ARG
1	D	2	ARG
1	D	20	LEU
1	D	21	LEU
1	D	28	ARG
1	D	44	GLU
1	D	50	LEU
1	D	56	LEU
1	D	64	ARG
1	D	79	GLN
1	D	80	GLU
1	D	100	ASP
1	D	104	THR
1	D	109	LEU
1	D	127	LEU
1	D	139	LEU
1	D	141	VAL
1	D	149	LEU
1	D	163	LEU

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Mol	Chain	Res	Type
1	D	171	ARG
1	E	2	ARG
1	E	6	CYS
1	E	10	LEU
1	E	20	LEU
1	E	25	ARG
1	E	33	LYS
1	E	50	LEU
1	E	56	LEU
1	E	57	LEU
1	E	100	ASP
1	E	101	LEU
1	E	104	THR
1	E	109	LEU
1	E	125	THR
1	E	127	LEU
1	E	139	LEU
1	E	141	VAL
1	E	148	ARG
1	E	149	LEU
1	E	151	GLU
1	E	157	ASP
1	E	163	LEU
1	E	164	ARG
1	E	171	ARG
1	E	175	GLU
1	E	189	LEU
1	F	10	LEU
1	F	20	LEU
1	F	25	ARG
1	F	28	ARG
1	F	43	VAL
1	F	56	LEU
1	F	57	LEU
1	F	68	GLU
1	F	69	ILE
1	F	109	LEU
1	F	118	GLU
1	F	121	ARG
1	F	125	THR
1	F	137	ARG
1	F	149	LEU

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Mol	Chain	Res	Type
1	F	153	THR
1	F	158	LYS
1	F	163	LEU
1	F	176	ARG
1	F	186	VAL
1	G	2	ARG
1	G	20	LEU
1	G	25	ARG
1	G	28	ARG
1	G	42	LYS
1	G	44	GLU
1	G	54	ILE
1	G	65	GLU
1	G	75	ASN
1	G	103	VAL
1	G	109	LEU
1	G	121	ARG
1	G	125	THR
1	G	139	LEU
1	G	141	VAL
1	G	151	GLU
1	G	160	VAL
1	G	161	SER
1	G	163	LEU
1	G	175	GLU
1	G	188	ARG
1	H	2	ARG
1	H	20	LEU
1	H	21	LEU
1	H	44	GLU
1	H	50	LEU
1	H	56	LEU
1	H	64	ARG
1	H	79	GLN
1	H	94	GLU
1	H	104	THR
1	H	109	LEU
1	H	127	LEU
1	H	139	LEU
1	H	140	GLU
1	H	141	VAL
1	H	149	LEU

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Mol	Chain	Res	Type
1	H	163	LEU
1	H	171	ARG
1	I	2	ARG
1	I	10	LEU
1	I	20	LEU
1	I	25	ARG
1	I	33	LYS
1	I	50	LEU
1	I	56	LEU
1	I	57	LEU
1	I	64	ARG
1	I	101	LEU
1	I	104	THR
1	I	125	THR
1	I	127	LEU
1	I	139	LEU
1	I	141	VAL
1	I	144	LYS
1	I	148	ARG
1	I	151	GLU
1	I	157	ASP
1	I	163	LEU
1	I	171	ARG
1	I	175	GLU
1	I	189	LEU
1	J	10	LEU
1	J	20	LEU
1	J	25	ARG
1	J	43	VAL
1	J	56	LEU
1	J	57	LEU
1	J	58	GLU
1	J	68	GLU
1	J	69	ILE
1	J	109	LEU
1	J	121	ARG
1	J	125	THR
1	J	148	ARG
1	J	149	LEU
1	J	153	THR
1	J	158	LYS
1	J	163	LEU

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Mol	Chain	Res	Type
1	J	176[A]	ARG
1	J	176[B]	ARG
1	J	186	VAL
1	J	190	ASN
1	K	2	ARG
1	K	20	LEU
1	K	22	LYS
1	K	25	ARG
1	K	26	GLU
1	K	28	ARG
1	K	42	LYS
1	K	54	ILE
1	K	75	ASN
1	K	103	VAL
1	K	109	LEU
1	K	121	ARG
1	K	139	LEU
1	K	141	VAL
1	K	151	GLU
1	K	160	VAL
1	K	161	SER
1	K	163	LEU
1	K	175	GLU
1	K	188	ARG
1	L	2	ARG
1	L	20	LEU
1	L	21	LEU
1	L	25	ARG
1	L	44	GLU
1	L	50	LEU
1	L	56	LEU
1	L	64	ARG
1	L	79	GLN
1	L	80	GLU
1	L	104	THR
1	L	109	LEU
1	L	127	LEU
1	L	139	LEU
1	L	141	VAL
1	L	149	LEU
1	L	163	LEU
1	L	164	ARG

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Mol	Chain	Res	Type
1	L	171	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	E	39	HIS
1	F	39	HIS
1	G	110	ASN
1	I	39	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	M	0/16	-	-
2	N	0/16	-	-
2	O	0/16	-	-
All	All	0/48	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 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 [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	190/199 (95%)	0.13	1 (0%) 91 80	29, 49, 82, 124	0
1	B	191/199 (95%)	0.07	2 (1%) 82 66	26, 45, 75, 110	0
1	C	189/199 (94%)	0.07	4 (2%) 63 43	29, 49, 82, 94	0
1	D	187/199 (93%)	-0.02	0 100 100	29, 56, 81, 98	0
1	E	190/199 (95%)	0.23	7 (3%) 41 25	31, 51, 81, 120	0
1	F	190/199 (95%)	0.20	1 (0%) 91 80	27, 47, 76, 108	0
1	G	189/199 (94%)	-0.08	0 100 100	30, 51, 80, 92	0
1	H	187/199 (93%)	-0.11	1 (0%) 91 80	30, 58, 82, 99	0
1	I	190/199 (95%)	0.33	10 (5%) 26 15	31, 51, 83, 121	0
1	J	190/199 (95%)	0.06	1 (0%) 91 80	25, 45, 76, 110	0
1	K	189/199 (94%)	-0.15	0 100 100	30, 50, 77, 98	0
1	L	187/199 (93%)	-0.14	1 (0%) 91 80	30, 58, 81, 94	0
2	M	15/16 (93%)	0.47	0 100 100	44, 72, 124, 129	3 (20%)
2	N	15/16 (93%)	0.51	1 (6%) 17 9	46, 73, 123, 130	3 (20%)
2	O	15/16 (93%)	0.59	2 (13%) 3 1	47, 74, 126, 128	3 (20%)
All	All	2314/2436 (94%)	0.06	31 (1%) 77 59	25, 51, 83, 130	9 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	1[B]	U	4.1
1	C	72	TYR	3.8
1	E	101	LEU	3.7
1	J	1	MET	3.3
1	I	101	LEU	3.2
1	I	98	GLU	2.9
1	F	13	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	159	LEU	2.8
1	C	186	VAL	2.7
1	I	99	ILE	2.6
2	O	2[A]	U	2.5
1	E	132	PHE	2.5
1	E	189	LEU	2.4
1	I	97	PHE	2.4
1	I	108	PHE	2.3
1	I	112	PHE	2.3
1	H	103	VAL	2.2
1	E	74	CYS	2.2
1	L	72	TYR	2.2
1	I	159	LEU	2.2
1	B	191	GLU	2.2
1	C	17	ARG	2.2
1	I	94	GLU	2.2
1	E	141	VAL	2.2
1	I	10	LEU	2.1
1	B	187	ALA	2.1
1	E	108	PHE	2.1
1	E	100	ASP	2.1
1	C	10	LEU	2.0
2	N	14[A]	A	2.0
1	I	139	LEU	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
4	CL	G	221	1/1	0.71	0.17	75,75,75,75	0
4	CL	K	221	1/1	0.89	0.14	87,87,87,87	0
4	CL	F	219	1/1	0.91	0.16	84,84,84,84	0
3	MG	H	197	1/1	0.92	0.14	59,59,59,59	0
4	CL	B	219	1/1	0.93	0.20	80,80,80,80	0
3	MG	K	197	1/1	0.93	0.15	54,54,54,54	0
3	MG	C	197	1/1	0.95	0.06	50,50,50,50	0
3	MG	D	197	1/1	0.95	0.05	64,64,64,64	0
3	MG	I	197	1/1	0.95	0.08	44,44,44,44	0
3	MG	L	197	1/1	0.95	0.08	63,63,63,63	0
3	MG	G	197	1/1	0.96	0.10	53,53,53,53	0
3	MG	A	197	1/1	0.97	0.09	42,42,42,42	0
3	MG	J	197	1/1	0.98	0.11	35,35,35,35	0
3	MG	F	197	1/1	0.98	0.11	34,34,34,34	0
3	MG	B	197	1/1	0.98	0.09	30,30,30,30	0
3	MG	E	197	1/1	0.99	0.09	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.