



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:10 pm GMT

PDB ID : 4OAY
Title : BldD CTD-c-di-GMP complex
Authors : Schumacher, M.A.; Tschowri, N.; Buttner, M.; Brennan, R.G.
Deposited on : 2014-01-06
Resolution : 1.95 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

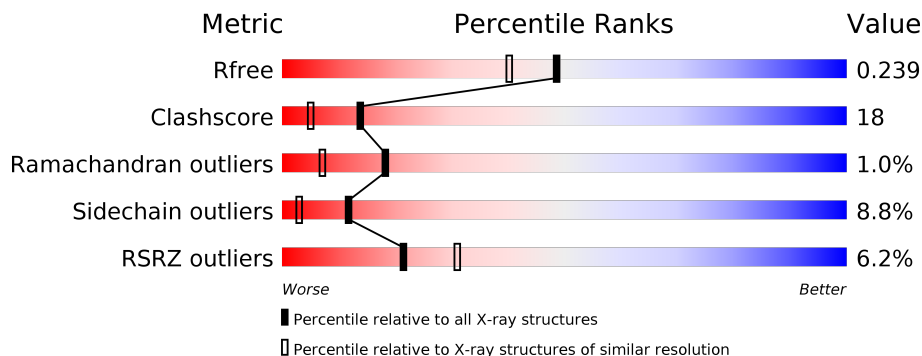
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	91	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	91	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>15%</div> <div>•</div> <div>20%</div> </div> </div>
1	D	91	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	91	<div> <div>5%</div> <div> <div></div> <div>48%</div> <div>30%</div> <div>• •</div> <div>16%</div> </div> </div>
1	F	91	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>20%</div> <div>•</div> <div>16%</div> </div> </div>
1	G	91	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>20%</div> <div>• •</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	H	91	<div><div></div><div>3%</div><div>56%</div><div>22%</div><div>5%</div><div>16%</div></div>
1	J	91	<div><div></div><div>4%</div><div>64%</div><div>20%</div><div>• •</div><div>13%</div></div>
1	K	91	<div><div></div><div>2%</div><div>59%</div><div>23%</div><div>• •</div><div>13%</div></div>
1	M	91	<div><div></div><div>16%</div><div>46%</div><div>30%</div><div>7%</div><div>•</div><div>16%</div></div>
1	N	91	<div><div></div><div>3%</div><div>60%</div><div>23%</div><div>•</div><div>13%</div></div>
1	R	91	<div><div></div><div>7%</div><div>69%</div><div>12%</div><div>• •</div><div>13%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16200 atoms, of which 7372 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 DNA-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	80	Total	C	H	N	O	Se	0	0	0
			1271	394	642	115	119	1			
1	B	73	Total	C	H	N	O	Se	0	0	0
			1161	362	586	102	110	1			
1	K	79	Total	C	H	N	O	Se	0	0	0
			1257	389	635	114	118	1			
1	J	79	Total	C	H	N	O	Se	0	0	0
			1257	389	635	114	118	1			
1	R	79	Total	C	H	N	O	Se	0	0	0
			1242	386	624	113	118	1			
1	H	76	Total	C	H	N	O	Se	0	0	0
			1192	372	597	107	115	1			
1	E	76	Total	C	H	N	O	Se	0	0	0
			1192	372	597	107	115	1			
1	G	76	Total	C	H	N	O	Se	0	0	0
			1192	372	597	107	115	1			
1	F	76	Total	C	H	N	O	Se	0	0	0
			1207	375	608	108	115	1			
1	D	79	Total	C	H	N	O	Se	0	0	0
			1242	386	624	113	118	1			
1	N	79	Total	C	H	N	O	Se	0	0	0
			1257	389	635	114	118	1			
1	M	76	Total	C	H	N	O	Se	0	0	0
			1190	375	591	108	115	1			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
A	77	SER	-	EXPRESSION TAG	UNP F2RCL8
A	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
A	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
A	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8

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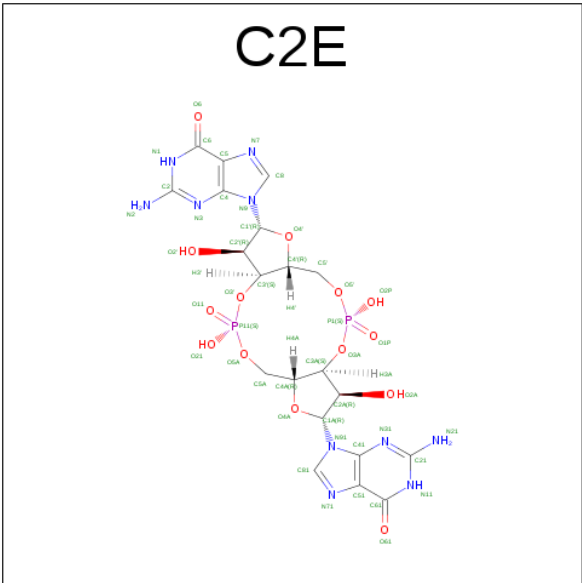
Chain	Residue	Modelled	Actual	Comment	Reference
B	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
B	77	SER	-	EXPRESSION TAG	UNP F2RCL8
B	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
B	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
B	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
K	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
K	77	SER	-	EXPRESSION TAG	UNP F2RCL8
K	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
K	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
K	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
J	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
J	77	SER	-	EXPRESSION TAG	UNP F2RCL8
J	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
J	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
J	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
R	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
R	77	SER	-	EXPRESSION TAG	UNP F2RCL8
R	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
R	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
R	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
H	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
H	77	SER	-	EXPRESSION TAG	UNP F2RCL8
H	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
H	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
H	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
E	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
E	77	SER	-	EXPRESSION TAG	UNP F2RCL8
E	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
E	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
E	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
G	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
G	77	SER	-	EXPRESSION TAG	UNP F2RCL8
G	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
G	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
G	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
F	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
F	77	SER	-	EXPRESSION TAG	UNP F2RCL8
F	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
F	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
F	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
D	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
D	77	SER	-	EXPRESSION TAG	UNP F2RCL8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
D	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
D	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
N	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
N	77	SER	-	EXPRESSION TAG	UNP F2RCL8
N	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
N	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
N	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8
M	76	GLY	-	EXPRESSION TAG	UNP F2RCL8
M	77	SER	-	EXPRESSION TAG	UNP F2RCL8
M	78	HIS	-	EXPRESSION TAG	UNP F2RCL8
M	79	MSE	-	EXPRESSION TAG	UNP F2RCL8
M	92	MSE	LEU	ENGINEERED MUTATION	UNP F2RCL8

- Molecule 2 is 9,9'-[(2R,3R,3AS,5S,7AR,9R,10R,10AS,12S,14AR)-3,5,10,12-TETRAHYDROXY-5,12-DIOXIDOOCTAHYDRO-2H,7H-DIFURO[3,2-D:3',2'-J][1,3,7,9,2,8]TETRAOXA DIPHOSPHACYCLODODECINE-2,9-DIYL]BIS(2-AMINO-1,9-DIHYDRO-6H-PURIN-6-ONE) (three-letter code: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	K	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	K	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	J	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	J	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	R	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	R	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	H	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	H	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	E	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	E	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	G	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	G	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	F	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	F	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	D	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	D	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	N	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	N	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	M	1	Total 46	C 20	N 10	O 14	P 2	0	0
2	M	1	Total 46	C 20	N 10	O 14	P 2	0	0

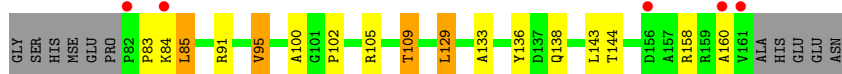
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	32	Total 32	O 32	0	0
3	K	53	Total 53	O 53	0	0
3	J	50	Total 50	O 50	0	0
3	R	58	Total 58	O 58	0	0
3	H	20	Total 20	O 20	0	0
3	E	26	Total 26	O 26	0	0
3	G	56	Total 56	O 56	0	0
3	F	27	Total 27	O 27	0	0
3	D	46	Total 46	O 46	0	0
3	N	34	Total 34	O 34	0	0
3	M	11	Total 11	O 11	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: DNA-binding protein



- Molecule 1: DNA-binding protein



- Molecule 1: DNA-binding protein



- Molecule 1: DNA-binding protein



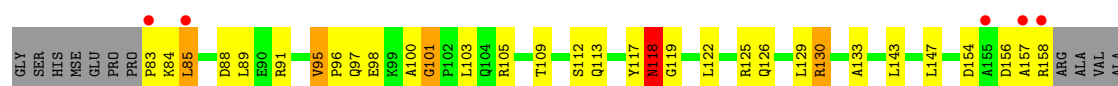
- Molecule 1: DNA-binding protein



- Molecule 1: DNA-binding protein



- Molecule 1: DNA-binding protein



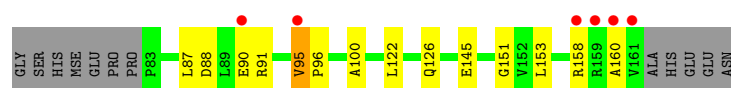
- Molecule 1: DNA-binding protein



- Molecule 1: DNA-binding protein



- Molecule 1: DNA-binding protein

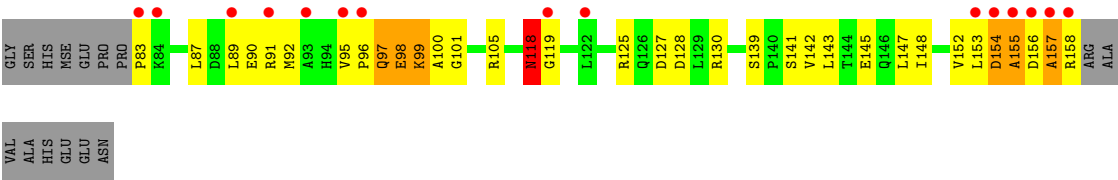


- Molecule 1: DNA-binding protein



- Molecule 1: DNA-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	86.50Å 86.50Å 151.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.91 – 1.95 74.91 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (74.91-1.95) 98.5 (74.91-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.198 , 0.234 0.210 , 0.239	Depositor DCC
R_{free} test set	2009 reflections (2.26%)	DCC
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.033 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16200	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C2E

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	0.71	0/638	0.88	0/864
1	B	0.79	0/583	0.87	1/789 (0.1%)
1	D	0.92	0/626	0.86	0/848
1	E	0.80	0/603	0.87	2/817 (0.2%)
1	F	0.82	1/607 (0.2%)	0.92	2/821 (0.2%)
1	G	1.02	1/603 (0.2%)	0.96	2/817 (0.2%)
1	H	0.81	0/603	0.80	1/817 (0.1%)
1	J	0.96	0/630	0.94	1/852 (0.1%)
1	K	0.94	2/630 (0.3%)	0.95	3/852 (0.4%)
1	M	0.75	0/607	0.81	0/821
1	N	0.95	0/630	0.95	1/852 (0.1%)
1	R	0.97	0/626	0.91	1/848 (0.1%)
All	All	0.88	4/7386 (0.1%)	0.90	14/9998 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	107	ALA	CA-CB	6.39	1.65	1.52
1	G	145	GLU	CG-CD	5.93	1.60	1.51
1	K	90	GLU	CB-CG	5.33	1.62	1.52
1	K	90	GLU	CG-CD	5.08	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	116	ASP	CB-CG-OD1	7.87	125.38	118.30
1	F	91	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	F	91	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	125	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	J	91	ARG	NE-CZ-NH1	6.66	123.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	105	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	R	91	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	E	105	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	K	114	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	K	85	LEU	CB-CG-CD1	-5.67	101.35	111.00
1	K	95	VAL	CB-CA-C	5.36	121.58	111.40
1	E	125	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	G	137	ASP	CB-CG-OD1	5.25	123.02	118.30
1	G	137	ASP	CB-CG-OD2	-5.20	113.62	118.30

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	629	642	641	14	0
1	B	575	586	585	13	0
1	D	618	624	623	12	0
1	E	595	597	596	35	1
1	F	599	608	607	21	0
1	G	595	597	596	20	0
1	H	595	597	596	31	1
1	J	622	635	634	24	1
1	K	622	635	634	21	0
1	M	599	591	607	41	0
1	N	622	635	634	22	0
1	R	618	624	623	17	0
2	A	91	1	38	5	0
2	B	92	0	39	3	0
2	D	92	0	41	3	0
2	E	92	0	41	1	0
2	F	92	0	44	2	0
2	G	92	0	41	3	0
2	H	92	0	41	1	0
2	J	92	0	41	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	92	0	41	4	0
2	M	92	0	39	4	0
2	N	92	0	40	3	0
2	R	92	0	43	0	0
3	A	23	0	0	1	0
3	B	32	0	0	1	2
3	D	46	0	0	2	0
3	E	26	0	0	9	0
3	F	27	0	0	4	2
3	G	56	0	0	8	0
3	H	20	0	0	5	0
3	J	50	0	0	2	0
3	K	53	0	0	4	0
3	M	11	0	0	2	0
3	N	34	0	0	7	0
3	R	58	0	0	4	1
All	All	8828	7372	7865	288	4

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 18.

All (288) 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:K:85:LEU:HD13	1:K:129:LEU:HD11	1.29	1.13
1:G:83:PRO:N	3:G:353:HOH:O	1.82	1.10
1:G:155:ALA:HB2	3:G:334:HOH:O	1.61	1.00
1:D:90:GLU:HB3	3:D:343:HOH:O	1.62	1.00
1:N:92:MSE:HE2	1:N:103:LEU:HD21	1.44	0.95
1:H:92:MSE:HE2	1:H:103:LEU:CG	1.97	0.95
1:H:88:ASP:OD1	3:H:315:HOH:O	1.87	0.93
1:K:85:LEU:HD13	1:K:129:LEU:CD1	1.99	0.93
1:R:113:GLN:NE2	3:R:320:HOH:O	1.91	0.92
1:K:137:ASP:OD1	3:K:351:HOH:O	1.87	0.92
1:R:83:PRO:N	3:R:358:HOH:O	2.01	0.91
1:F:97:GLN:OE1	3:F:322:HOH:O	1.89	0.91
1:M:83:PRO:HB2	1:M:157:ALA:HA	1.51	0.90
1:G:155:ALA:CB	3:G:334:HOH:O	2.18	0.90
1:E:83:PRO:CA	3:E:317:HOH:O	2.19	0.89
1:M:97:GLN:HG3	1:M:98:GLU:N	1.86	0.88
2:M:202:C2E:O2P	3:M:308:HOH:O	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:ALA:N	3:G:334:HOH:O	2.02	0.87
1:J:84:LYS:HE2	3:J:333:HOH:O	1.74	0.86
1:D:95:VAL:HG22	1:D:100:ALA:HB2	1.60	0.84
1:N:91:ARG:HH11	1:N:91:ARG:HB3	1.41	0.84
1:K:95:VAL:HG22	1:K:100:ALA:HB2	1.60	0.83
1:E:83:PRO:N	3:E:317:HOH:O	2.13	0.81
1:H:92:MSE:HE2	1:H:103:LEU:HG	1.63	0.81
1:E:85:LEU:HD21	1:E:129:LEU:HD12	1.62	0.80
1:H:92:MSE:HE2	1:H:103:LEU:CD2	2.12	0.80
1:A:83:PRO:HG2	1:A:160:ALA:HB2	1.64	0.80
1:H:147:LEU:HD12	1:H:153:LEU:HD22	1.62	0.80
1:R:127:ASP:HB3	3:R:324:HOH:O	1.82	0.79
1:K:92:MSE:HE2	1:K:103:LEU:CD1	2.14	0.78
1:N:159:ARG:NH2	3:N:331:HOH:O	2.12	0.78
1:B:84:LYS:HB3	1:B:86:VAL:HG23	1.65	0.78
1:H:92:MSE:HE2	1:H:103:LEU:HD21	1.66	0.77
1:A:105:ARG:O	1:A:109:THR:HG22	1.85	0.76
1:E:95:VAL:HG23	1:E:96:PRO:HD2	1.66	0.76
1:R:91:ARG:HD3	1:R:150:TRP:O	1.86	0.76
1:M:148:ILE:HD13	1:M:155:ALA:HA	1.69	0.75
1:N:92:MSE:HE2	1:N:103:LEU:CD2	2.17	0.75
1:E:130:ARG:NH1	3:E:305:HOH:O	2.19	0.75
1:H:105:ARG:NH1	3:H:311:HOH:O	2.18	0.74
1:N:126:GLN:OE1	1:N:160:ALA:HB1	1.88	0.74
1:K:87:LEU:HD13	1:K:92:MSE:HE1	1.70	0.74
1:K:92:MSE:HE2	1:K:103:LEU:HD11	1.70	0.74
1:H:156:ASP:OD2	3:H:316:HOH:O	2.07	0.73
1:F:90:GLU:HA	1:F:90:GLU:OE1	1.88	0.73
1:E:118:ASN:CG	1:E:119:GLY:H	1.93	0.72
1:D:95:VAL:HG22	1:D:100:ALA:CB	2.19	0.72
1:E:83:PRO:HB2	1:E:157:ALA:O	1.90	0.72
1:M:98:GLU:N	1:M:98:GLU:OE1	2.23	0.72
2:A:201:C2E:N3	2:A:201:C2E:N1	2.37	0.71
1:M:97:GLN:O	1:M:99:LYS:N	2.24	0.70
1:K:85:LEU:CD1	1:K:129:LEU:CD1	2.69	0.70
1:D:95:VAL:CG2	1:D:100:ALA:HB2	2.21	0.69
1:M:95:VAL:HG23	1:M:96:PRO:HD2	1.74	0.68
2:A:201:C2E:N2	2:A:201:C2E:N3	2.41	0.68
1:J:129:LEU:O	1:J:129:LEU:HD13	1.92	0.68
1:F:97:GLN:NE2	3:F:322:HOH:O	2.25	0.68
1:E:95:VAL:HG22	1:E:100:ALA:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:GLU:OE1	1:J:158:ARG:NH1	2.27	0.67
1:M:156:ASP:O	1:M:158:ARG:N	2.27	0.67
2:A:201:C2E:N2	2:A:201:C2E:N1	2.43	0.67
1:J:138:GLN:HB3	1:J:142:VAL:HG13	1.76	0.67
1:E:83:PRO:HA	3:E:317:HOH:O	1.86	0.66
1:F:105:ARG:NH2	3:F:326:HOH:O	2.29	0.66
1:H:146:GLN:NE2	1:H:150:TRP:CZ2	2.64	0.66
1:M:95:VAL:HG13	1:M:100:ALA:CB	2.26	0.65
1:E:83:PRO:O	1:E:85:LEU:HD13	1.97	0.65
1:G:130:ARG:NE	3:G:356:HOH:O	2.03	0.64
1:F:87:LEU:HD23	1:F:153:LEU:HD13	1.80	0.64
1:M:118:ASN:CG	1:M:119:GLY:N	2.50	0.64
1:J:83:PRO:HG3	1:J:160:ALA:N	2.12	0.64
1:G:130:ARG:NH2	3:G:356:HOH:O	2.26	0.63
1:E:83:PRO:HD2	1:E:126:GLN:HE22	1.62	0.63
1:H:92:MSE:CE	1:H:103:LEU:HD11	2.29	0.63
1:N:159:ARG:NH1	3:N:331:HOH:O	2.32	0.62
1:H:146:GLN:CG	1:H:150:TRP:CZ2	2.83	0.62
1:B:97:GLN:O	1:B:98:GLU:C	2.36	0.62
1:E:85:LEU:HD21	1:E:129:LEU:CD1	2.29	0.62
1:N:87:LEU:HD23	1:N:153:LEU:HD13	1.81	0.62
1:J:138:GLN:HB3	1:J:142:VAL:CG1	2.30	0.61
1:N:87:LEU:HD13	1:N:92:MSE:HE1	1.81	0.61
1:R:130:ARG:H	1:R:130:ARG:HD2	1.63	0.61
1:G:156:ASP:O	1:G:158:ARG:N	2.33	0.61
1:H:87:LEU:HD23	1:H:153:LEU:HD13	1.82	0.61
1:K:92:MSE:HE2	1:K:103:LEU:HD13	1.83	0.61
1:K:105:ARG:O	1:K:109:THR:HG23	2.01	0.60
1:M:97:GLN:HG3	1:M:98:GLU:H	1.65	0.60
1:N:84:LYS:HE2	3:N:329:HOH:O	2.00	0.60
1:J:161:VAL:O	1:J:161:VAL:HG22	2.00	0.60
1:M:99:LYS:HA	1:M:99:LYS:HE3	1.82	0.59
1:E:83:PRO:HB2	1:E:157:ALA:C	2.23	0.59
1:J:87:LEU:HD23	1:J:153:LEU:HD13	1.85	0.59
1:J:129:LEU:C	1:J:129:LEU:HD13	2.23	0.59
1:F:118:ASN:HD21	1:F:121:VAL:H	1.50	0.58
1:K:127:ASP:OD2	3:K:309:HOH:O	2.16	0.58
1:D:91:ARG:HD2	1:D:151:GLY:O	2.04	0.57
1:E:129:LEU:CD2	1:E:143:LEU:HD12	2.34	0.57
1:M:99:LYS:CE	1:M:99:LYS:HA	2.33	0.57
1:H:92:MSE:HE2	1:H:103:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:VAL:HG23	1:E:96:PRO:CD	2.34	0.57
1:H:146:GLN:NE2	1:H:150:TRP:HZ2	2.03	0.57
1:H:90:GLU:HB3	3:H:315:HOH:O	2.04	0.56
1:J:126:GLN:NE2	1:J:160:ALA:HB1	2.20	0.56
1:F:86:VAL:O	1:F:153:LEU:HD12	2.05	0.56
2:K:201:C2E:O21	3:K:302:HOH:O	2.18	0.56
1:R:83:PRO:HG3	1:R:160:ALA:N	2.20	0.56
1:E:129:LEU:HD23	1:E:143:LEU:HD12	1.88	0.56
1:H:147:LEU:CD1	1:H:153:LEU:HD22	2.31	0.56
1:J:87:LEU:HD23	1:J:153:LEU:CD1	2.35	0.56
1:K:126:GLN:OE1	1:K:160:ALA:HB1	2.06	0.56
1:M:97:GLN:C	1:M:99:LYS:N	2.59	0.56
1:N:91:ARG:NH1	1:N:91:ARG:HB3	2.15	0.55
1:A:95:VAL:HG22	1:A:100:ALA:HB2	1.88	0.55
1:A:83:PRO:HG3	1:A:160:ALA:N	2.21	0.55
1:M:118:ASN:CG	1:M:119:GLY:H	2.10	0.55
1:E:118:ASN:CG	1:E:119:GLY:N	2.60	0.55
1:M:92:MSE:O	1:M:95:VAL:HG12	2.07	0.54
1:G:125:ARG:HG2	2:G:201:C2E:H8	1.90	0.54
1:J:83:PRO:CG	1:J:160:ALA:HA	2.37	0.54
1:N:84:LYS:HE3	2:N:201:C2E:O3'	2.08	0.54
1:K:85:LEU:CD1	1:K:129:LEU:HD13	2.38	0.54
1:M:83:PRO:HB2	1:M:157:ALA:CA	2.30	0.54
1:D:145:GLU:OE2	1:D:158:ARG:CD	2.55	0.54
1:G:130:ARG:NH1	3:G:307:HOH:O	2.28	0.53
1:R:129:LEU:HB3	1:R:130:ARG:HE	1.72	0.53
1:R:85:LEU:N	1:R:85:LEU:CD1	2.70	0.53
1:E:83:PRO:CB	1:E:157:ALA:O	2.56	0.53
1:K:125:ARG:HG2	2:K:201:C2E:H8	1.90	0.53
1:B:147:LEU:HB2	1:B:153:LEU:HD12	1.91	0.53
1:K:84:LYS:HE2	3:K:308:HOH:O	2.07	0.53
1:G:155:ALA:CA	3:G:334:HOH:O	2.41	0.53
1:R:132:LEU:HB3	1:R:143:LEU:HD21	1.91	0.53
1:D:126:GLN:OE1	1:D:160:ALA:HB1	2.09	0.53
1:J:91:ARG:HD2	1:J:150:TRP:O	2.08	0.53
1:G:118:ASN:CG	1:G:119:GLY:N	2.62	0.53
1:R:83:PRO:HG2	1:R:160:ALA:HB2	1.90	0.53
1:F:97:GLN:CD	3:F:322:HOH:O	2.34	0.52
1:B:147:LEU:CB	1:B:153:LEU:HD12	2.40	0.52
1:F:125:ARG:HG2	2:F:201:C2E:H8	1.92	0.52
1:H:85:LEU:HD13	1:H:129:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:TYR:O	1:E:118:ASN:O	2.27	0.52
1:M:95:VAL:HG13	1:M:100:ALA:HB2	1.91	0.52
1:R:155:ALA:HB2	3:R:342:HOH:O	2.09	0.52
1:F:133:ALA:HB1	1:F:138:GLN:O	2.10	0.52
1:E:83:PRO:O	1:E:85:LEU:CD1	2.58	0.52
1:N:130:ARG:HD2	3:N:305:HOH:O	2.09	0.52
1:F:118:ASN:OD1	1:F:118:ASN:C	2.48	0.51
1:G:87:LEU:HD23	1:G:153:LEU:HD13	1.90	0.51
1:D:95:VAL:HG23	1:D:96:PRO:HD2	1.92	0.51
1:D:87:LEU:HD23	1:D:153:LEU:HD13	1.92	0.51
1:M:83:PRO:CB	1:M:157:ALA:O	2.59	0.51
1:F:123:SER:OG	2:F:202:C2E:N7	2.42	0.51
1:M:141:SER:O	1:M:145:GLU:HG2	2.10	0.51
1:H:92:MSE:HE2	1:H:103:LEU:HD11	1.92	0.51
1:M:89:LEU:HD12	1:M:119:GLY:HA2	1.92	0.51
1:E:83:PRO:HG3	1:E:158:ARG:O	2.11	0.51
1:M:127:ASP:OD2	1:M:130:ARG:NH1	2.43	0.51
1:H:139:SER:OG	1:H:142:VAL:HG23	2.11	0.50
2:D:202:C2E:O21	3:D:302:HOH:O	2.19	0.50
1:H:106:TYR:CE2	1:H:110:ILE:HD11	2.47	0.50
1:M:125:ARG:O	1:M:128:ASP:HB2	2.11	0.50
1:M:95:VAL:CG2	1:M:96:PRO:HD2	2.41	0.50
1:N:143:LEU:C	1:N:143:LEU:HD13	2.31	0.50
1:B:101:GLY:O	1:B:105:ARG:HG3	2.12	0.50
1:F:85:LEU:CD1	1:F:85:LEU:N	2.74	0.50
1:K:95:VAL:HG22	1:K:100:ALA:CB	2.38	0.50
1:M:125:ARG:HG2	2:M:201:C2E:H8	1.94	0.50
1:J:91:ARG:CD	1:J:150:TRP:O	2.59	0.49
1:N:159:ARG:CZ	3:N:331:HOH:O	2.52	0.49
1:E:85:LEU:N	1:E:85:LEU:HD13	2.27	0.49
1:H:92:MSE:HE1	1:H:103:LEU:HD11	1.94	0.49
1:M:95:VAL:CG1	1:M:100:ALA:HB2	2.43	0.49
1:A:84:LYS:HE2	3:A:304:HOH:O	2.12	0.49
1:E:91:ARG:NH1	3:E:321:HOH:O	2.46	0.49
1:J:83:PRO:HG3	1:J:160:ALA:HA	1.95	0.49
1:M:139:SER:OG	1:M:142:VAL:HG23	2.13	0.49
1:K:84:LYS:HE3	2:K:201:C2E:O3'	2.13	0.49
1:J:130:ARG:NH1	3:J:340:HOH:O	2.23	0.48
1:H:147:LEU:HD12	1:H:153:LEU:CD2	2.38	0.48
1:J:83:PRO:HG3	1:J:160:ALA:CA	2.42	0.48
1:N:84:LYS:HD3	3:N:311:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:ASN:HD21	1:F:121:VAL:HG12	1.78	0.48
1:N:87:LEU:HD23	1:N:153:LEU:CD1	2.45	0.47
1:H:146:GLN:HG2	1:H:150:TRP:CZ2	2.49	0.47
1:R:87:LEU:HD23	1:R:153:LEU:HD13	1.96	0.47
1:J:92:MSE:HG3	1:J:103:LEU:HD13	1.96	0.47
1:K:153:LEU:HG	1:K:157:ALA:HB2	1.96	0.47
1:D:145:GLU:OE2	1:D:158:ARG:HD2	2.14	0.47
2:B:202:C2E:H5'2	2:B:202:C2E:H512	1.97	0.47
1:D:88:ASP:OD2	1:D:91:ARG:HG3	2.15	0.47
2:E:202:C2E:H5'2	2:E:202:C2E:H512	1.97	0.47
1:N:125:ARG:HG2	2:N:201:C2E:H8	1.97	0.47
1:J:83:PRO:CG	1:J:160:ALA:CA	2.93	0.47
2:N:202:C2E:H512	2:N:202:C2E:H5'2	1.97	0.46
1:J:139:SER:O	1:J:142:VAL:HG12	2.16	0.46
2:M:202:C2E:H512	2:M:202:C2E:H5'2	1.97	0.46
1:M:87:LEU:HD23	1:M:153:LEU:HD13	1.98	0.46
2:K:202:C2E:H512	2:K:202:C2E:H5'2	1.97	0.46
1:N:155:ALA:O	1:N:158:ARG:HG3	2.15	0.46
1:A:133:ALA:HB1	1:A:138:GLN:O	2.14	0.46
1:H:92:MSE:CE	1:H:103:LEU:HG	2.42	0.46
2:D:201:C2E:H5'2	2:D:201:C2E:H512	1.97	0.46
1:E:130:ARG:HG2	3:E:310:HOH:O	2.16	0.46
1:M:89:LEU:HD12	1:M:119:GLY:CA	2.46	0.46
1:H:138:GLN:OE1	1:H:143:LEU:HD23	2.15	0.46
2:B:202:C2E:N71	3:B:328:HOH:O	2.36	0.46
1:G:129:LEU:CD2	1:G:143:LEU:HD12	2.45	0.46
1:G:83:PRO:CB	1:G:157:ALA:HA	2.46	0.46
1:B:132:LEU:HB3	1:B:143:LEU:HD21	1.96	0.46
1:E:84:LYS:N	3:E:317:HOH:O	2.48	0.46
1:G:133:ALA:HB1	1:G:138:GLN:O	2.15	0.45
2:H:202:C2E:H512	2:H:202:C2E:H5'2	1.97	0.45
1:M:156:ASP:C	1:M:158:ARG:N	2.70	0.45
2:G:202:C2E:H512	2:G:202:C2E:H5'2	1.97	0.45
1:M:97:GLN:O	1:M:98:GLU:C	2.54	0.45
1:N:146:GLN:NE2	3:N:320:HOH:O	2.44	0.45
2:M:202:C2E:P1	3:M:308:HOH:O	2.71	0.45
1:H:92:MSE:CE	1:H:103:LEU:HD21	2.42	0.45
2:A:202:C2E:H512	2:A:202:C2E:H5'2	1.97	0.45
1:A:85:LEU:N	1:A:85:LEU:CD1	2.79	0.45
1:F:136:TYR:O	1:F:138:GLN:HG3	2.16	0.45
1:B:85:LEU:HG	1:B:126:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:LEU:HG	1:G:157:ALA:HB2	1.98	0.45
1:B:125:ARG:HG2	2:B:201:C2E:H8	2.00	0.44
1:M:83:PRO:CB	1:M:157:ALA:HA	2.34	0.44
1:E:89:LEU:HD21	1:E:122:LEU:HB3	1.98	0.44
1:B:97:GLN:O	1:B:99:LYS:N	2.51	0.44
1:A:129:LEU:CD1	1:A:144:THR:OG1	2.65	0.44
1:M:89:LEU:CD1	1:M:119:GLY:HA2	2.48	0.43
1:A:83:PRO:CG	1:A:160:ALA:HB2	2.42	0.43
1:E:100:ALA:O	1:E:101:GLY:C	2.57	0.43
1:E:85:LEU:CD1	1:E:85:LEU:N	2.82	0.43
1:H:153:LEU:HD12	1:H:153:LEU:HA	1.86	0.43
1:E:109:THR:O	1:E:113:GLN:HG3	2.19	0.43
1:K:158:ARG:O	1:K:161:VAL:HG12	2.18	0.43
1:K:84:LYS:HB3	1:K:86:VAL:HG23	2.01	0.43
1:R:147:LEU:HB3	1:R:153:LEU:HB2	2.00	0.43
1:M:154:ASP:OD1	1:M:155:ALA:N	2.51	0.43
1:F:86:VAL:CG1	1:F:121:VAL:HG23	2.49	0.43
1:H:84:LYS:HE2	3:H:318:HOH:O	2.19	0.43
1:M:147:LEU:HA	1:M:147:LEU:HD23	1.81	0.43
1:M:97:GLN:O	1:M:100:ALA:N	2.52	0.43
1:A:102:PRO:HB2	1:A:136:TYR:CE1	2.54	0.43
1:B:84:LYS:HB3	1:B:86:VAL:CG2	2.43	0.43
1:G:83:PRO:HG2	1:G:158:ARG:O	2.18	0.43
1:H:146:GLN:HG3	1:H:150:TRP:CE2	2.52	0.43
1:A:83:PRO:O	1:A:85:LEU:HD13	2.19	0.42
1:N:140:PRO:HB2	1:N:161:VAL:HG21	2.00	0.42
1:E:97:GLN:HG3	1:E:97:GLN:O	2.19	0.42
1:F:158:ARG:HH11	1:F:158:ARG:CB	2.32	0.42
1:R:130:ARG:N	1:R:130:ARG:HD2	2.30	0.42
1:M:154:ASP:O	1:M:156:ASP:N	2.52	0.42
1:R:83:PRO:HG3	1:R:160:ALA:H	1.83	0.42
1:G:83:PRO:HB3	1:G:157:ALA:HA	2.01	0.42
1:F:155:ALA:HB1	1:F:158:ARG:HH12	1.84	0.42
1:H:92:MSE:CE	1:H:103:LEU:CD1	2.94	0.42
1:M:89:LEU:HD12	1:M:119:GLY:C	2.40	0.42
1:H:84:LYS:HA	1:H:84:LYS:HD2	1.78	0.42
1:E:88:ASP:CG	1:E:91:ARG:HG3	2.40	0.42
1:R:83:PRO:CG	1:R:160:ALA:N	2.83	0.42
1:J:126:GLN:HE22	1:J:160:ALA:HB1	1.84	0.41
1:N:92:MSE:HE2	1:N:103:LEU:CG	2.50	0.41
1:J:129:LEU:C	1:J:129:LEU:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:83:PRO:HD2	1:R:160:ALA:HA	2.02	0.41
1:D:95:VAL:HA	1:D:96:PRO:HD3	1.87	0.41
1:B:146:GLN:HG3	1:B:150:TRP:CZ2	2.56	0.41
1:F:142:VAL:O	1:F:142:VAL:HG12	2.19	0.41
1:N:147:LEU:HD12	1:N:153:LEU:HD22	2.02	0.41
1:J:85:LEU:HD21	1:J:160:ALA:CB	2.51	0.41
1:B:132:LEU:CB	1:B:143:LEU:HD21	2.51	0.41
1:E:83:PRO:CB	1:E:157:ALA:C	2.88	0.41
1:J:114:ARG:HG2	2:D:202:C2E:H81	2.01	0.41
1:M:101:GLY:O	1:M:105:ARG:HG3	2.20	0.41
1:M:97:GLN:C	1:M:99:LYS:H	2.24	0.41
1:A:143:LEU:HD13	1:A:143:LEU:C	2.40	0.40
1:F:86:VAL:CG1	1:F:121:VAL:CG2	2.98	0.40
1:E:147:LEU:HD23	1:E:147:LEU:HA	1.74	0.40
3:E:326:HOH:O	1:F:84:LYS:HE2	2.20	0.40
1:G:117:TYR:O	1:G:118:ASN:C	2.59	0.40
1:K:91:ARG:HA	1:K:91:ARG:HD3	1.90	0.40
1:A:84:LYS:HE3	2:A:201:C2E:O3'	2.21	0.40
1:B:97:GLN:C	1:B:99:LYS:N	2.74	0.40
1:M:95:VAL:CG1	1:M:100:ALA:CB	2.97	0.40
1:M:83:PRO:HB2	1:M:157:ALA:O	2.20	0.40
1:E:133:ALA:HB3	3:E:310:HOH:O	2.21	0.40
1:A:91:ARG:HA	1:A:91:ARG:HD3	1.97	0.40
1:E:118:ASN:ND2	1:E:119:GLY:H	2.19	0.40
1:G:125:ARG:CG	2:G:201:C2E:H8	2.51	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:304:HOH:O	3:F:308:HOH:O[1_545]	1.72	0.48
3:B:327:HOH:O	3:F:308:HOH:O[1_545]	1.80	0.40
1:H:113:GLN:HE21	1:E:130:ARG:HH21[1_445]	1.31	0.29
1:J:127:ASP:OD1	3:R:325:HOH:O[1_455]	1.92	0.28

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	78/91 (86%)	77 (99%)	1 (1%)	0	100	100
1	B	71/91 (78%)	67 (94%)	3 (4%)	1 (1%)	13	4
1	D	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
1	E	74/91 (81%)	69 (93%)	3 (4%)	2 (3%)	6	1
1	F	74/91 (81%)	73 (99%)	1 (1%)	0	100	100
1	G	74/91 (81%)	70 (95%)	2 (3%)	2 (3%)	6	1
1	H	74/91 (81%)	71 (96%)	3 (4%)	0	100	100
1	J	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
1	K	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
1	M	74/91 (81%)	68 (92%)	2 (3%)	4 (5%)	2	0
1	N	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
1	R	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
All	All	904/1092 (83%)	871 (96%)	24 (3%)	9 (1%)	18	7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	118	ASN
1	G	157	ALA
1	M	98	GLU
1	M	118	ASN
1	M	157	ALA
1	B	98	GLU
1	E	101	GLY
1	M	155	ALA
1	G	118	ASN

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	68/75 (91%)	63 (93%)	5 (7%)	16	5
1	B	63/75 (84%)	59 (94%)	4 (6%)	21	8
1	D	66/75 (88%)	64 (97%)	2 (3%)	46	34
1	E	64/75 (85%)	55 (86%)	9 (14%)	4	1
1	F	65/75 (87%)	59 (91%)	6 (9%)	11	3
1	G	64/75 (85%)	59 (92%)	5 (8%)	15	4
1	H	64/75 (85%)	56 (88%)	8 (12%)	5	1
1	J	67/75 (89%)	64 (96%)	3 (4%)	32	17
1	K	67/75 (89%)	62 (92%)	5 (8%)	16	5
1	M	65/75 (87%)	57 (88%)	8 (12%)	5	1
1	N	67/75 (89%)	59 (88%)	8 (12%)	6	1
1	R	66/75 (88%)	60 (91%)	6 (9%)	11	3
All	All	786/900 (87%)	717 (91%)	69 (9%)	12	3

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	95	VAL
1	A	109	THR
1	A	129	LEU
1	A	158	ARG
1	B	84	LYS
1	B	97	GLN
1	B	129	LEU
1	B	141	SER
1	K	95	VAL
1	K	103	LEU
1	K	153	LEU
1	K	154	ASP
1	K	156	ASP

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Mol	Chain	Res	Type
1	J	91	ARG
1	J	103	LEU
1	J	153	LEU
1	R	85	LEU
1	R	91	ARG
1	R	129	LEU
1	R	130	ARG
1	R	153	LEU
1	R	156	ASP
1	H	84	LYS
1	H	127	ASP
1	H	129	LEU
1	H	130	ARG
1	H	143	LEU
1	H	145	GLU
1	H	153	LEU
1	H	154	ASP
1	E	85	LEU
1	E	95	VAL
1	E	98	GLU
1	E	103	LEU
1	E	112	SER
1	E	118	ASN
1	E	130	ARG
1	E	154	ASP
1	E	156	ASP
1	G	84	LYS
1	G	97	GLN
1	G	105	ARG
1	G	118	ASN
1	G	129	LEU
1	F	90	GLU
1	F	91	ARG
1	F	103	LEU
1	F	118	ASN
1	F	153	LEU
1	F	156	ASP
1	D	95	VAL
1	D	122	LEU
1	N	91	ARG
1	N	97	GLN
1	N	127	ASP

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Mol	Chain	Res	Type
1	N	129	LEU
1	N	130	ARG
1	N	153	LEU
1	N	154	ASP
1	N	156	ASP
1	M	90	GLU
1	M	91	ARG
1	M	97	GLN
1	M	99	LYS
1	M	118	ASN
1	M	143	LEU
1	M	152	VAL
1	M	154	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	94	HIS
1	K	138	GLN
1	J	126	GLN
1	H	94	HIS
1	E	126	GLN
1	G	97	GLN
1	M	146	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C2E	A	201	-	41,49,52	2.38	10 (24%)	45,77,82	2.23	12 (26%)
2	C2E	A	202	-	44,52,52	2.47	14 (31%)	50,82,82	2.29	14 (28%)
2	C2E	B	201	-	44,52,52	2.45	16 (36%)	50,82,82	3.04	26 (52%)
2	C2E	B	202	-	44,52,52	2.46	14 (31%)	50,82,82	2.30	14 (28%)
2	C2E	D	201	-	44,52,52	2.47	14 (31%)	50,82,82	2.29	15 (30%)
2	C2E	D	202	-	44,52,52	2.37	11 (25%)	50,82,82	2.40	15 (30%)
2	C2E	E	201	-	44,52,52	2.37	11 (25%)	50,82,82	2.40	15 (30%)
2	C2E	E	202	-	44,52,52	2.46	14 (31%)	50,82,82	2.29	15 (30%)
2	C2E	F	201	-	44,52,52	2.46	11 (25%)	50,82,82	2.60	19 (38%)
2	C2E	F	202	-	44,52,52	2.52	12 (27%)	50,82,82	1.95	12 (24%)
2	C2E	G	201	-	44,52,52	2.74	19 (43%)	50,82,82	2.65	18 (36%)
2	C2E	G	202	-	44,52,52	2.46	13 (29%)	50,82,82	2.29	15 (30%)
2	C2E	H	201	-	44,52,52	2.37	11 (25%)	50,82,82	2.40	15 (30%)
2	C2E	H	202	-	44,52,52	2.47	13 (29%)	50,82,82	2.29	14 (28%)
2	C2E	J	201	-	44,52,52	2.92	19 (43%)	50,82,82	2.73	24 (48%)
2	C2E	J	202	-	44,52,52	2.61	16 (36%)	50,82,82	2.72	19 (38%)
2	C2E	K	201	-	44,52,52	2.37	11 (25%)	50,82,82	2.40	15 (30%)
2	C2E	K	202	-	44,52,52	2.46	14 (31%)	50,82,82	2.29	14 (28%)
2	C2E	M	201	-	44,52,52	2.58	20 (45%)	50,82,82	2.93	19 (38%)
2	C2E	M	202	-	44,52,52	2.46	13 (29%)	50,82,82	2.29	14 (28%)
2	C2E	N	201	-	44,52,52	2.70	20 (45%)	50,82,82	2.87	19 (38%)
2	C2E	N	202	-	44,52,52	2.47	14 (31%)	50,82,82	2.29	14 (28%)
2	C2E	R	201	-	44,52,52	2.64	17 (38%)	50,82,82	2.83	22 (44%)
2	C2E	R	202	-	44,52,52	2.52	12 (27%)	50,82,82	1.95	12 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C2E	A	201	-	-	0/22/62/62	0/5/6/7
2	C2E	A	202	-	-	0/22/62/62	0/6/7/7
2	C2E	B	201	-	-	0/22/62/62	0/6/7/7
2	C2E	B	202	-	-	0/22/62/62	0/6/7/7
2	C2E	D	201	-	-	0/22/62/62	0/6/7/7
2	C2E	D	202	-	-	0/22/62/62	0/6/7/7
2	C2E	E	201	-	-	0/22/62/62	0/6/7/7
2	C2E	E	202	-	-	0/22/62/62	0/6/7/7
2	C2E	F	201	-	-	0/22/62/62	0/6/7/7
2	C2E	F	202	-	-	0/22/62/62	0/6/7/7
2	C2E	G	201	-	-	0/22/62/62	0/6/7/7
2	C2E	G	202	-	-	0/22/62/62	0/6/7/7
2	C2E	H	201	-	-	0/22/62/62	0/6/7/7
2	C2E	H	202	-	-	0/22/62/62	0/6/7/7
2	C2E	J	201	-	-	0/22/62/62	0/6/7/7
2	C2E	J	202	-	-	0/22/62/62	0/6/7/7
2	C2E	K	201	-	-	0/22/62/62	0/6/7/7
2	C2E	K	202	-	-	0/22/62/62	0/6/7/7
2	C2E	M	201	-	-	0/22/62/62	0/6/7/7
2	C2E	M	202	-	-	0/22/62/62	0/6/7/7
2	C2E	N	201	-	-	0/22/62/62	0/6/7/7
2	C2E	N	202	-	-	0/22/62/62	0/6/7/7
2	C2E	R	201	-	-	0/22/62/62	0/6/7/7
2	C2E	R	202	-	-	0/22/62/62	0/6/7/7

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	202	C2E	C2'-C1'	-7.60	1.41	1.53
2	H	202	C2E	C2'-C1'	-7.58	1.41	1.53
2	D	201	C2E	C2'-C1'	-7.57	1.41	1.53
2	N	202	C2E	C2'-C1'	-7.57	1.41	1.53
2	G	202	C2E	C2'-C1'	-7.55	1.41	1.53
2	A	202	C2E	C2'-C1'	-7.55	1.41	1.53
2	B	202	C2E	C2'-C1'	-7.53	1.41	1.53
2	M	202	C2E	C2'-C1'	-7.53	1.41	1.53
2	K	202	C2E	C2'-C1'	-7.53	1.41	1.53
2	F	202	C2E	C2'-C1'	-7.00	1.42	1.53
2	R	202	C2E	C2'-C1'	-6.94	1.42	1.53
2	A	201	C2E	C2'-C1'	-6.62	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	201	C2E	C2'-C1'	-6.60	1.43	1.53
2	H	201	C2E	C2'-C1'	-6.59	1.43	1.53
2	D	202	C2E	C2'-C1'	-6.58	1.43	1.53
2	E	201	C2E	C2'-C1'	-6.55	1.43	1.53
2	R	202	C2E	C8-N7	-6.54	1.22	1.34
2	F	202	C2E	C8-N7	-6.53	1.22	1.34
2	A	201	C2E	C8-N7	-6.23	1.23	1.35
2	G	201	C2E	C2'-C1'	-6.22	1.43	1.53
2	B	202	C2E	C2'-C3'	-6.06	1.39	1.53
2	M	202	C2E	C2'-C3'	-6.05	1.39	1.53
2	A	202	C2E	C2'-C3'	-6.05	1.39	1.53
2	G	202	C2E	C2'-C3'	-6.05	1.39	1.53
2	D	201	C2E	C2'-C3'	-6.04	1.39	1.53
2	N	202	C2E	C2'-C3'	-6.03	1.39	1.53
2	E	202	C2E	C2'-C3'	-6.03	1.39	1.53
2	H	202	C2E	C2'-C3'	-6.02	1.39	1.53
2	K	202	C2E	C2'-C3'	-6.00	1.39	1.53
2	H	201	C2E	C8-N7	-5.85	1.23	1.34
2	E	201	C2E	C8-N7	-5.83	1.23	1.34
2	J	201	C2E	O2'-C2'	-5.82	1.29	1.43
2	D	202	C2E	C8-N7	-5.82	1.23	1.34
2	K	201	C2E	C8-N7	-5.81	1.23	1.34
2	F	202	C2E	C2'-C3'	-5.76	1.40	1.53
2	M	201	C2E	C2'-C1'	-5.74	1.44	1.53
2	R	202	C2E	C2'-C3'	-5.73	1.40	1.53
2	F	201	C2E	C2'-C1'	-5.72	1.44	1.53
2	F	201	C2E	C81-N71	-5.60	1.24	1.34
2	R	201	C2E	C2'-C1'	-5.45	1.45	1.53
2	F	201	C2E	C8-N7	-5.42	1.24	1.34
2	J	202	C2E	C2'-C1'	-5.40	1.45	1.53
2	R	202	C2E	C81-N71	-5.15	1.25	1.34
2	F	202	C2E	C81-N71	-5.12	1.25	1.34
2	N	201	C2E	C2'-C1'	-5.08	1.45	1.53
2	M	202	C2E	C81-N71	-4.97	1.25	1.34
2	H	202	C2E	C81-N71	-4.96	1.25	1.34
2	N	202	C2E	C81-N71	-4.96	1.25	1.34
2	D	201	C2E	C81-N71	-4.95	1.25	1.34
2	E	202	C2E	C81-N71	-4.94	1.25	1.34
2	B	202	C2E	C81-N71	-4.93	1.25	1.34
2	K	202	C2E	C81-N71	-4.92	1.25	1.34
2	A	202	C2E	C81-N71	-4.91	1.25	1.34
2	G	202	C2E	C81-N71	-4.89	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	C2E	C2'-C3'	-4.79	1.42	1.53
2	E	201	C2E	C2'-C3'	-4.74	1.42	1.53
2	D	202	C2E	C2'-C3'	-4.73	1.42	1.53
2	A	201	C2E	C2'-C3'	-4.73	1.42	1.53
2	K	201	C2E	C2'-C3'	-4.73	1.42	1.53
2	M	201	C2E	O2'-C2'	-4.62	1.32	1.43
2	J	201	C2E	C2'-C1'	-4.56	1.46	1.53
2	B	201	C2E	O2'-C2'	-4.51	1.32	1.43
2	A	201	C2E	C81-N71	-4.34	1.26	1.34
2	E	201	C2E	C81-N71	-4.33	1.26	1.34
2	N	201	C2E	O2'-C2'	-4.33	1.33	1.43
2	K	201	C2E	C81-N71	-4.32	1.26	1.34
2	D	202	C2E	C81-N71	-4.32	1.26	1.34
2	H	201	C2E	C81-N71	-4.31	1.26	1.34
2	M	201	C2E	C51-C41	-4.28	1.30	1.40
2	G	201	C2E	C2'-C3'	-4.27	1.43	1.53
2	F	201	C2E	C2'-C3'	-4.24	1.43	1.53
2	G	202	C2E	C8-N7	-4.17	1.26	1.34
2	G	201	C2E	O2'-C2'	-4.16	1.33	1.43
2	B	202	C2E	C8-N7	-4.15	1.26	1.34
2	H	202	C2E	C8-N7	-4.15	1.26	1.34
2	A	202	C2E	C8-N7	-4.14	1.26	1.34
2	K	202	C2E	C8-N7	-4.14	1.26	1.34
2	D	201	C2E	C8-N7	-4.14	1.26	1.34
2	M	202	C2E	C8-N7	-4.14	1.26	1.34
2	J	202	C2E	C2'-C3'	-4.13	1.43	1.53
2	N	202	C2E	C8-N7	-4.13	1.26	1.34
2	E	202	C2E	C8-N7	-4.12	1.27	1.34
2	G	201	C2E	C51-C41	-4.10	1.31	1.40
2	B	201	C2E	C2'-C1'	-4.09	1.47	1.53
2	A	201	C2E	C5-C6	-4.08	1.39	1.51
2	R	201	C2E	C51-C41	-4.05	1.31	1.40
2	J	202	C2E	O2'-C2'	-4.04	1.33	1.43
2	N	201	C2E	C2'-C3'	-3.93	1.44	1.53
2	R	201	C2E	O2'-C2'	-3.92	1.33	1.43
2	N	201	C2E	C8-N7	-3.85	1.27	1.34
2	N	201	C2E	C51-C41	-3.82	1.31	1.40
2	N	201	C2E	C5-C4	-3.75	1.32	1.40
2	B	201	C2E	C8-N7	-3.73	1.27	1.34
2	J	201	C2E	C51-C41	-3.72	1.32	1.40
2	J	201	C2E	O4A-C1A	-3.69	1.36	1.41
2	J	201	C2E	C2'-C3'	-3.59	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	C2E	C5-C4	-3.58	1.32	1.40
2	N	201	C2E	O4'-C1'	-3.52	1.36	1.41
2	B	201	C2E	C5-C4	-3.30	1.33	1.40
2	J	201	C2E	C2A-C1A	-3.30	1.48	1.53
2	F	201	C2E	O4'-C4'	-3.26	1.37	1.45
2	R	201	C2E	C2A-C1A	-3.20	1.48	1.53
2	N	201	C2E	C81-N71	-3.07	1.28	1.34
2	J	202	C2E	O4A-C1A	-3.06	1.37	1.41
2	G	201	C2E	O4A-C1A	-3.04	1.37	1.41
2	B	201	C2E	C51-C41	-3.02	1.33	1.40
2	B	201	C2E	C81-N71	-2.99	1.29	1.34
2	J	201	C2E	C8-N7	-2.96	1.29	1.34
2	J	202	C2E	C81-N71	-2.87	1.29	1.34
2	B	201	C2E	C2'-C3'	-2.87	1.46	1.53
2	M	201	C2E	C2A-C1A	-2.85	1.49	1.53
2	B	202	C2E	O2A-C2A	-2.82	1.36	1.43
2	M	202	C2E	O2A-C2A	-2.82	1.36	1.43
2	N	202	C2E	O2A-C2A	-2.81	1.36	1.43
2	A	202	C2E	O2A-C2A	-2.81	1.36	1.43
2	D	201	C2E	O2A-C2A	-2.81	1.36	1.43
2	M	202	C2E	P11-O3'	-2.80	1.53	1.60
2	B	202	C2E	P11-O3'	-2.79	1.53	1.60
2	G	202	C2E	O2A-C2A	-2.79	1.36	1.43
2	N	202	C2E	P11-O3'	-2.79	1.53	1.60
2	E	202	C2E	P11-O3'	-2.78	1.53	1.60
2	A	202	C2E	P11-O3'	-2.78	1.53	1.60
2	K	202	C2E	O2A-C2A	-2.78	1.36	1.43
2	E	202	C2E	O2A-C2A	-2.77	1.36	1.43
2	K	202	C2E	P11-O3'	-2.76	1.53	1.60
2	N	201	C2E	O2A-C2A	-2.76	1.36	1.43
2	H	202	C2E	O2A-C2A	-2.76	1.36	1.43
2	G	202	C2E	P11-O3'	-2.76	1.53	1.60
2	H	202	C2E	P11-O3'	-2.76	1.53	1.60
2	D	201	C2E	P11-O3'	-2.75	1.53	1.60
2	M	201	C2E	C2'-C3'	-2.69	1.47	1.53
2	J	202	C2E	C2A-C1A	-2.68	1.49	1.53
2	J	201	C2E	O2A-C2A	-2.65	1.36	1.43
2	R	201	C2E	C5-C4	-2.64	1.34	1.40
2	M	201	C2E	C8-N7	-2.62	1.29	1.34
2	F	202	C2E	C2A-C1A	-2.59	1.49	1.53
2	M	201	C2E	O4A-C4A	-2.59	1.39	1.45
2	F	201	C2E	O2A-C2A	-2.59	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	C2E	O4A-C4A	-2.58	1.39	1.45
2	R	202	C2E	C2A-C1A	-2.56	1.49	1.53
2	G	201	C2E	O4A-C4A	-2.55	1.39	1.45
2	N	201	C2E	C2A-C1A	-2.55	1.49	1.53
2	M	201	C2E	C81-N71	-2.55	1.29	1.34
2	M	201	C2E	O5'-C5'	-2.53	1.34	1.44
2	R	201	C2E	C2'-C3'	-2.51	1.47	1.53
2	F	202	C2E	P11-O3'	-2.42	1.54	1.60
2	R	202	C2E	P11-O3'	-2.41	1.54	1.60
2	J	202	C2E	C8-N7	-2.40	1.30	1.34
2	K	201	C2E	O2A-C2A	-2.38	1.37	1.43
2	A	201	C2E	O2A-C2A	-2.38	1.37	1.43
2	H	201	C2E	O2A-C2A	-2.36	1.37	1.43
2	D	202	C2E	O2A-C2A	-2.36	1.37	1.43
2	M	201	C2E	C5-C4	-2.35	1.35	1.40
2	E	201	C2E	O2A-C2A	-2.34	1.37	1.43
2	G	201	C2E	C81-N71	-2.31	1.30	1.34
2	R	201	C2E	C81-N71	-2.30	1.30	1.34
2	B	201	C2E	O4A-C1A	-2.29	1.38	1.41
2	J	201	C2E	C81-N71	-2.27	1.30	1.34
2	G	201	C2E	C2A-C3A	-2.27	1.48	1.53
2	R	202	C2E	P11-O11	-2.25	1.42	1.50
2	F	202	C2E	P11-O11	-2.24	1.42	1.50
2	J	202	C2E	C51-C41	-2.21	1.35	1.40
2	J	201	C2E	C5-C4	-2.18	1.35	1.40
2	N	202	C2E	O5A-C5A	-2.17	1.36	1.44
2	K	202	C2E	O5A-C5A	-2.17	1.36	1.44
2	R	201	C2E	O2A-C2A	-2.16	1.38	1.43
2	M	202	C2E	O5A-C5A	-2.16	1.36	1.44
2	A	202	C2E	O5A-C5A	-2.16	1.36	1.44
2	H	202	C2E	O5A-C5A	-2.16	1.36	1.44
2	D	201	C2E	O5A-C5A	-2.15	1.36	1.44
2	G	201	C2E	C8-N7	-2.15	1.30	1.34
2	N	201	C2E	O4'-C4'	-2.15	1.40	1.45
2	G	202	C2E	O5A-C5A	-2.15	1.36	1.44
2	J	201	C2E	O4'-C4'	-2.15	1.40	1.45
2	B	202	C2E	O5A-C5A	-2.15	1.36	1.44
2	E	202	C2E	O5A-C5A	-2.14	1.36	1.44
2	G	201	C2E	O4'-C4'	-2.09	1.40	1.45
2	H	201	C2E	O5'-C5'	-2.08	1.36	1.44
2	E	201	C2E	O5'-C5'	-2.08	1.36	1.44
2	K	201	C2E	O5'-C5'	-2.07	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	C2E	O5'-C5'	-2.06	1.36	1.44
2	D	202	C2E	O5'-C5'	-2.06	1.36	1.44
2	E	202	C2E	O5'-C5'	-2.03	1.36	1.44
2	D	201	C2E	O5'-C5'	-2.03	1.36	1.44
2	M	201	C2E	C2A-C3A	-2.02	1.48	1.53
2	N	202	C2E	O5'-C5'	-2.02	1.36	1.44
2	K	202	C2E	O5'-C5'	-2.01	1.36	1.44
2	A	202	C2E	O5'-C5'	-2.00	1.36	1.44
2	B	202	C2E	O5'-C5'	-2.00	1.36	1.44
2	M	201	C2E	P11-O11	2.02	1.58	1.50
2	M	202	C2E	O2'-C2'	2.07	1.47	1.43
2	K	202	C2E	O2'-C2'	2.07	1.47	1.43
2	G	202	C2E	O2'-C2'	2.08	1.47	1.43
2	E	202	C2E	O2'-C2'	2.08	1.47	1.43
2	N	202	C2E	O2'-C2'	2.08	1.47	1.43
2	H	202	C2E	O2'-C2'	2.09	1.47	1.43
2	A	202	C2E	O2'-C2'	2.10	1.47	1.43
2	D	201	C2E	O2'-C2'	2.11	1.47	1.43
2	B	202	C2E	O2'-C2'	2.11	1.47	1.43
2	R	201	C2E	C61-N11	2.12	1.36	1.33
2	G	201	C2E	C61-N11	2.15	1.36	1.33
2	G	201	C2E	C6-N1	2.17	1.37	1.33
2	G	202	C2E	C51-C41	2.28	1.45	1.40
2	N	201	C2E	C61-N11	2.29	1.37	1.33
2	E	202	C2E	C51-C41	2.29	1.45	1.40
2	D	201	C2E	C51-C41	2.30	1.45	1.40
2	K	202	C2E	C51-C41	2.30	1.45	1.40
2	H	202	C2E	C51-C41	2.31	1.45	1.40
2	A	202	C2E	C51-C41	2.31	1.45	1.40
2	M	201	C2E	C6-N1	2.32	1.37	1.33
2	B	202	C2E	C51-C41	2.32	1.45	1.40
2	M	202	C2E	C51-C41	2.32	1.45	1.40
2	N	202	C2E	C51-C41	2.33	1.45	1.40
2	N	201	C2E	C61-C51	2.41	1.46	1.41
2	R	202	C2E	O4A-C4A	2.42	1.50	1.45
2	J	201	C2E	C2-N1	2.46	1.39	1.35
2	N	201	C2E	C2-N1	2.46	1.39	1.35
2	F	202	C2E	O4A-C4A	2.48	1.50	1.45
2	R	202	C2E	C61-N11	2.48	1.37	1.33
2	F	202	C2E	C61-N11	2.50	1.37	1.33
2	F	201	C2E	C5-C4	2.53	1.46	1.40
2	H	201	C2E	C5-C4	2.54	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	202	C2E	C5-C4	2.55	1.46	1.40
2	H	202	C2E	C5-C4	2.56	1.46	1.40
2	B	202	C2E	C5-C4	2.56	1.46	1.40
2	G	202	C2E	C5-C4	2.56	1.46	1.40
2	D	202	C2E	C5-C4	2.56	1.46	1.40
2	E	202	C2E	C5-C4	2.57	1.46	1.40
2	D	201	C2E	C5-C4	2.58	1.46	1.40
2	A	202	C2E	C5-C4	2.58	1.46	1.40
2	K	201	C2E	C5-C4	2.59	1.46	1.40
2	E	201	C2E	C5-C4	2.59	1.46	1.40
2	N	202	C2E	C5-C4	2.60	1.46	1.40
2	K	202	C2E	C5-C4	2.61	1.46	1.40
2	J	202	C2E	C21-N11	2.63	1.40	1.35
2	B	201	C2E	C61-C51	2.64	1.46	1.41
2	F	201	C2E	O61-C61	2.70	1.31	1.24
2	B	201	C2E	C6-C5	2.71	1.46	1.41
2	R	201	C2E	C2-N1	2.74	1.40	1.35
2	J	202	C2E	C2-N1	2.79	1.40	1.35
2	M	201	C2E	C61-C51	2.87	1.46	1.41
2	H	201	C2E	O61-C61	2.88	1.31	1.24
2	A	201	C2E	O61-C61	2.89	1.31	1.24
2	E	201	C2E	O61-C61	2.91	1.31	1.24
2	K	201	C2E	O61-C61	2.91	1.31	1.24
2	D	202	C2E	O61-C61	2.91	1.31	1.24
2	R	201	C2E	C6-N1	2.97	1.38	1.33
2	N	201	C2E	C21-N11	3.02	1.40	1.35
2	R	201	C2E	C6-C5	3.05	1.47	1.41
2	F	202	C2E	O6-C6	3.05	1.32	1.24
2	N	201	C2E	C6-N1	3.05	1.38	1.33
2	R	202	C2E	O6-C6	3.08	1.32	1.24
2	B	201	C2E	C4-N3	3.11	1.40	1.35
2	B	201	C2E	C6-N1	3.18	1.38	1.33
2	M	201	C2E	C2-N1	3.30	1.41	1.35
2	M	201	C2E	C6-C5	3.32	1.47	1.41
2	R	201	C2E	C61-C51	3.40	1.47	1.41
2	R	201	C2E	C21-N11	3.42	1.41	1.35
2	H	201	C2E	O6-C6	3.49	1.33	1.24
2	M	202	C2E	O6-C6	3.49	1.33	1.24
2	N	202	C2E	O6-C6	3.50	1.33	1.24
2	K	201	C2E	O6-C6	3.50	1.33	1.24
2	B	202	C2E	O6-C6	3.50	1.33	1.24
2	J	202	C2E	C6-N1	3.51	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201	C2E	C21-N11	3.51	1.41	1.35
2	E	202	C2E	O6-C6	3.51	1.33	1.24
2	H	202	C2E	O6-C6	3.51	1.33	1.24
2	E	201	C2E	O6-C6	3.51	1.33	1.24
2	G	201	C2E	C6-C5	3.52	1.48	1.41
2	D	201	C2E	O6-C6	3.52	1.33	1.24
2	A	202	C2E	O6-C6	3.52	1.33	1.24
2	G	202	C2E	O6-C6	3.53	1.33	1.24
2	D	202	C2E	O6-C6	3.53	1.33	1.24
2	M	201	C2E	C4-N3	3.53	1.41	1.35
2	K	202	C2E	O6-C6	3.54	1.33	1.24
2	J	201	C2E	C6-C5	3.58	1.48	1.41
2	G	201	C2E	C21-N11	3.71	1.42	1.35
2	N	201	C2E	C6-C5	3.72	1.48	1.41
2	K	202	C2E	C21-N21	3.75	1.41	1.34
2	G	201	C2E	C61-C51	3.75	1.48	1.41
2	B	202	C2E	C21-N21	3.76	1.41	1.34
2	E	202	C2E	C21-N21	3.76	1.41	1.34
2	N	202	C2E	C21-N21	3.78	1.41	1.34
2	A	202	C2E	C21-N21	3.78	1.41	1.34
2	M	202	C2E	C21-N21	3.78	1.41	1.34
2	G	202	C2E	C21-N21	3.79	1.41	1.34
2	H	202	C2E	C21-N21	3.79	1.41	1.34
2	J	202	C2E	C6-C5	3.81	1.48	1.41
2	G	201	C2E	C4-N3	3.81	1.41	1.35
2	D	201	C2E	C21-N21	3.82	1.41	1.34
2	J	201	C2E	C6-N1	3.84	1.40	1.33
2	M	201	C2E	C21-N11	4.02	1.42	1.35
2	J	202	C2E	C61-N11	4.02	1.40	1.33
2	E	201	C2E	C21-N21	4.17	1.42	1.34
2	K	201	C2E	C21-N21	4.17	1.42	1.34
2	D	202	C2E	C21-N21	4.18	1.42	1.34
2	H	201	C2E	C21-N21	4.19	1.42	1.34
2	A	201	C2E	C21-N21	4.21	1.42	1.34
2	N	201	C2E	C4-N3	4.22	1.42	1.35
2	J	202	C2E	C4-N3	4.25	1.42	1.35
2	J	201	C2E	C61-N11	4.37	1.41	1.33
2	A	201	C2E	O6-C6	4.44	1.33	1.24
2	J	201	C2E	C4-N3	4.45	1.42	1.35
2	M	201	C2E	C21-N21	4.50	1.43	1.34
2	R	201	C2E	C4-N3	4.52	1.43	1.35
2	F	201	C2E	O6-C6	4.58	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	C2E	C21-N21	4.81	1.43	1.34
2	B	201	C2E	C21-N11	4.82	1.44	1.35
2	R	202	C2E	C21-N21	4.90	1.44	1.34
2	F	202	C2E	C21-N21	4.91	1.44	1.34
2	J	201	C2E	C21-N21	5.08	1.44	1.34
2	F	201	C2E	C21-N21	5.13	1.44	1.34
2	F	202	C2E	C2-N2	5.17	1.44	1.34
2	R	202	C2E	C2-N2	5.20	1.44	1.34
2	N	201	C2E	C21-N21	5.27	1.44	1.34
2	J	202	C2E	C21-N21	5.30	1.44	1.34
2	G	201	C2E	C21-N21	5.46	1.45	1.34
2	G	202	C2E	C2-N2	5.79	1.45	1.34
2	B	202	C2E	C2-N2	5.80	1.45	1.34
2	M	202	C2E	C2-N2	5.82	1.46	1.34
2	N	202	C2E	C2-N2	5.82	1.46	1.34
2	H	202	C2E	C2-N2	5.84	1.46	1.34
2	K	202	C2E	C2-N2	5.84	1.46	1.34
2	D	201	C2E	C2-N2	5.84	1.46	1.34
2	A	202	C2E	C2-N2	5.84	1.46	1.34
2	E	202	C2E	C2-N2	5.85	1.46	1.34
2	D	202	C2E	C2-N2	6.16	1.46	1.34
2	H	201	C2E	C2-N2	6.17	1.46	1.34
2	K	201	C2E	C2-N2	6.17	1.46	1.34
2	F	201	C2E	C2-N2	6.18	1.46	1.34
2	E	201	C2E	C2-N2	6.19	1.46	1.34
2	R	201	C2E	C21-N21	6.40	1.47	1.34
2	M	201	C2E	C41-N31	7.16	1.47	1.35
2	B	201	C2E	C41-N31	7.49	1.47	1.35
2	N	201	C2E	C41-N31	7.85	1.48	1.35
2	J	202	C2E	C41-N31	7.95	1.48	1.35
2	G	201	C2E	C41-N31	8.54	1.49	1.35
2	R	201	C2E	C41-N31	8.84	1.50	1.35
2	J	201	C2E	C41-N31	10.24	1.52	1.35

All (391) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	C2E	C41-C51-N71	-6.58	103.05	109.41
2	G	201	C2E	N31-C21-N11	-6.57	117.86	127.46
2	D	202	C2E	C41-C51-N71	-6.49	103.14	109.41
2	E	201	C2E	C41-C51-N71	-6.48	103.15	109.41
2	H	201	C2E	C41-C51-N71	-6.47	103.16	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	201	C2E	C41-C51-N71	-6.45	103.18	109.41
2	A	201	C2E	C41-C51-N71	-6.44	103.19	109.41
2	B	201	C2E	N31-C21-N11	-6.28	118.29	127.46
2	F	202	C2E	C61-C51-C41	-6.25	114.63	120.84
2	M	201	C2E	N31-C21-N11	-6.24	118.34	127.46
2	F	201	C2E	C4A-O4A-C1A	-6.24	103.13	109.77
2	R	202	C2E	C61-C51-C41	-6.23	114.64	120.84
2	N	201	C2E	C51-C61-N11	-6.22	114.62	123.48
2	M	202	C2E	C41-C51-N71	-6.00	103.61	109.41
2	B	202	C2E	C41-C51-N71	-5.97	103.64	109.41
2	H	202	C2E	C41-C51-N71	-5.97	103.64	109.41
2	D	201	C2E	C41-C51-N71	-5.96	103.65	109.41
2	A	202	C2E	C41-C51-N71	-5.96	103.65	109.41
2	N	202	C2E	C41-C51-N71	-5.96	103.66	109.41
2	K	201	C2E	C6-C5-C4	-5.95	114.92	120.84
2	E	202	C2E	C41-C51-N71	-5.95	103.66	109.41
2	R	201	C2E	N31-C21-N11	-5.95	118.77	127.46
2	G	202	C2E	C41-C51-N71	-5.94	103.67	109.41
2	E	201	C2E	C6-C5-C4	-5.94	114.94	120.84
2	D	202	C2E	C6-C5-C4	-5.93	114.94	120.84
2	K	202	C2E	C41-C51-N71	-5.92	103.69	109.41
2	N	201	C2E	C2A-C3A-C4A	-5.89	92.69	103.23
2	H	201	C2E	C6-C5-C4	-5.85	115.02	120.84
2	B	201	C2E	C51-C61-N11	-5.85	115.15	123.48
2	J	202	C2E	C51-C61-N11	-5.83	115.18	123.48
2	N	201	C2E	N31-C21-N11	-5.81	118.97	127.46
2	N	201	C2E	C2'-C3'-C4'	-5.80	92.86	103.23
2	J	201	C2E	C5-C6-N1	-5.78	115.25	123.48
2	K	201	C2E	C2'-C3'-C4'	-5.75	92.94	103.23
2	D	202	C2E	C2'-C3'-C4'	-5.75	92.94	103.23
2	E	201	C2E	C2'-C3'-C4'	-5.75	92.94	103.23
2	H	201	C2E	C2'-C3'-C4'	-5.75	92.95	103.23
2	A	201	C2E	C2'-C3'-C4'	-5.74	92.96	103.23
2	R	202	C2E	C4-C5-N7	-5.72	103.88	109.41
2	F	202	C2E	C4-C5-N7	-5.72	103.89	109.41
2	B	201	C2E	C2'-C3'-C4'	-5.68	93.08	103.23
2	J	201	C2E	N31-C21-N11	-5.65	119.20	127.46
2	R	201	C2E	C2'-C3'-C4'	-5.63	93.15	103.23
2	A	202	C2E	C4-C5-N7	-5.52	104.08	109.41
2	K	202	C2E	C4-C5-N7	-5.52	104.08	109.41
2	N	202	C2E	C4-C5-N7	-5.51	104.08	109.41
2	G	201	C2E	C51-C61-N11	-5.51	115.64	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	C2E	C4-C5-N7	-5.48	104.11	109.41
2	J	201	C2E	C2'-C3'-C4'	-5.48	93.43	103.23
2	E	202	C2E	C4-C5-N7	-5.47	104.13	109.41
2	B	202	C2E	C4-C5-N7	-5.46	104.13	109.41
2	H	202	C2E	C4-C5-N7	-5.46	104.14	109.41
2	G	202	C2E	C4-C5-N7	-5.45	104.15	109.41
2	M	202	C2E	C4-C5-N7	-5.44	104.15	109.41
2	R	201	C2E	C51-C61-N11	-5.14	116.16	123.48
2	R	201	C2E	C5-C6-N1	-5.09	116.23	123.48
2	J	202	C2E	C5-C6-N1	-5.05	116.30	123.48
2	J	201	C2E	C51-C61-N11	-5.03	116.32	123.48
2	M	201	C2E	C5-C6-N1	-4.96	116.42	123.48
2	M	201	C2E	C51-C61-N11	-4.86	116.57	123.48
2	F	201	C2E	C4'-O4'-C1'	-4.76	104.71	109.77
2	J	202	C2E	N31-C21-N11	-4.70	120.60	127.46
2	K	201	C2E	C61-C51-C41	-4.70	116.17	120.84
2	D	202	C2E	C61-C51-C41	-4.69	116.18	120.84
2	F	201	C2E	C4-C5-N7	-4.68	104.88	109.41
2	A	201	C2E	C61-C51-C41	-4.68	116.19	120.84
2	F	201	C2E	C61-C51-C41	-4.68	116.19	120.84
2	G	201	C2E	N3-C2-N1	-4.67	120.65	127.46
2	E	201	C2E	C61-C51-C41	-4.66	116.21	120.84
2	G	201	C2E	C6-C5-C4	-4.66	116.22	120.84
2	H	201	C2E	C61-C51-C41	-4.65	116.22	120.84
2	B	201	C2E	N3-C2-N1	-4.63	120.70	127.46
2	F	201	C2E	C6-C5-C4	-4.35	116.52	120.84
2	G	201	C2E	C61-C51-C41	-4.33	116.54	120.84
2	M	201	C2E	C2'-C3'-C4'	-4.15	95.81	103.23
2	B	202	C2E	C6-C5-C4	-4.13	116.74	120.84
2	G	202	C2E	C6-C5-C4	-4.13	116.74	120.84
2	K	202	C2E	C6-C5-C4	-4.11	116.75	120.84
2	H	202	C2E	C6-C5-C4	-4.11	116.75	120.84
2	N	202	C2E	C6-C5-C4	-4.09	116.77	120.84
2	D	201	C2E	C6-C5-C4	-4.07	116.79	120.84
2	A	202	C2E	C6-C5-C4	-4.07	116.80	120.84
2	E	202	C2E	C6-C5-C4	-4.07	116.80	120.84
2	M	202	C2E	C6-C5-C4	-4.06	116.80	120.84
2	B	201	C2E	C5-C6-N1	-4.06	117.70	123.48
2	K	202	C2E	C61-C51-C41	-3.92	116.94	120.84
2	B	201	C2E	C6-C5-C4	-3.92	116.95	120.84
2	B	201	C2E	C4'-O4'-C1'	-3.91	105.60	109.77
2	E	202	C2E	C61-C51-C41	-3.89	116.97	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	201	C2E	C4'-O4'-C1'	-3.89	105.62	109.77
2	H	202	C2E	C61-C51-C41	-3.89	116.97	120.84
2	N	202	C2E	C61-C51-C41	-3.88	116.98	120.84
2	B	202	C2E	C61-C51-C41	-3.88	116.98	120.84
2	A	202	C2E	C61-C51-C41	-3.86	117.01	120.84
2	N	201	C2E	C6-C5-C4	-3.86	117.01	120.84
2	D	201	C2E	C61-C51-C41	-3.85	117.01	120.84
2	G	202	C2E	C61-C51-C41	-3.84	117.02	120.84
2	M	202	C2E	C61-C51-C41	-3.84	117.02	120.84
2	F	202	C2E	C4A-O4A-C1A	-3.82	105.70	109.77
2	R	202	C2E	C4A-O4A-C1A	-3.80	105.73	109.77
2	G	201	C2E	C5-C6-N1	-3.71	118.20	123.48
2	R	201	C2E	C6-C5-C4	-3.70	117.16	120.84
2	R	202	C2E	C6-C5-C4	-3.69	117.17	120.84
2	F	202	C2E	C6-C5-C4	-3.66	117.20	120.84
2	N	201	C2E	N3-C2-N1	-3.66	122.11	127.46
2	M	201	C2E	C61-C51-C41	-3.57	117.30	120.84
2	M	201	C2E	N3-C2-N1	-3.51	122.34	127.46
2	J	201	C2E	C61-C51-C41	-3.49	117.38	120.84
2	N	201	C2E	C61-C51-C41	-3.49	117.38	120.84
2	F	201	C2E	N31-C21-N11	-3.46	122.40	127.46
2	J	202	C2E	C4A-O4A-C1A	-3.46	106.08	109.77
2	F	201	C2E	N3-C2-N1	-3.45	122.42	127.46
2	R	201	C2E	C61-C51-C41	-3.45	117.42	120.84
2	D	202	C2E	C1'-N9-C4	-3.44	120.69	126.64
2	E	201	C2E	C1'-N9-C4	-3.43	120.70	126.64
2	K	201	C2E	C1'-N9-C4	-3.43	120.71	126.64
2	H	201	C2E	C1'-N9-C4	-3.41	120.75	126.64
2	R	201	C2E	N3-C2-N1	-3.38	122.53	127.46
2	N	202	C2E	C4A-O4A-C1A	-3.31	106.24	109.77
2	A	202	C2E	C4A-O4A-C1A	-3.31	106.24	109.77
2	K	202	C2E	C4A-O4A-C1A	-3.31	106.25	109.77
2	B	202	C2E	C4A-O4A-C1A	-3.30	106.25	109.77
2	E	202	C2E	C4A-O4A-C1A	-3.29	106.27	109.77
2	G	202	C2E	C4A-O4A-C1A	-3.29	106.27	109.77
2	H	202	C2E	C4A-O4A-C1A	-3.28	106.27	109.77
2	M	202	C2E	C4A-O4A-C1A	-3.28	106.28	109.77
2	J	202	C2E	N3-C2-N1	-3.27	122.69	127.46
2	D	201	C2E	C4A-O4A-C1A	-3.25	106.31	109.77
2	J	201	C2E	C2A-C3A-C4A	-3.18	97.54	103.23
2	H	201	C2E	C4-C5-N7	-3.17	106.34	109.41
2	K	201	C2E	C4-C5-N7	-3.15	106.37	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	C2E	C4-C5-N7	-3.14	106.37	109.41
2	E	201	C2E	C4-C5-N7	-3.13	106.39	109.41
2	B	201	C2E	C61-C51-C41	-3.12	117.75	120.84
2	M	202	C2E	C5-C6-N1	-3.08	119.11	123.48
2	N	201	C2E	C5-C6-N1	-3.07	119.11	123.48
2	D	202	C2E	N3-C2-N1	-3.07	122.98	127.46
2	H	201	C2E	N3-C2-N1	-3.06	122.99	127.46
2	H	201	C2E	C51-C61-N11	-3.05	119.14	123.48
2	E	201	C2E	N3-C2-N1	-3.05	123.00	127.46
2	R	202	C2E	N31-C21-N11	-3.05	123.01	127.46
2	H	202	C2E	C5-C6-N1	-3.05	119.14	123.48
2	N	202	C2E	C5-C6-N1	-3.05	119.15	123.48
2	A	201	C2E	C51-C61-N11	-3.05	119.15	123.48
2	K	201	C2E	N3-C2-N1	-3.04	123.01	127.46
2	E	202	C2E	C5-C6-N1	-3.04	119.15	123.48
2	B	202	C2E	C5-C6-N1	-3.04	119.15	123.48
2	K	201	C2E	C51-C61-N11	-3.04	119.16	123.48
2	F	202	C2E	N31-C21-N11	-3.04	123.03	127.46
2	G	202	C2E	C5-C6-N1	-3.03	119.16	123.48
2	D	202	C2E	C51-C61-N11	-3.03	119.17	123.48
2	K	202	C2E	C5-C6-N1	-3.03	119.17	123.48
2	D	201	C2E	C5-C6-N1	-3.03	119.17	123.48
2	A	202	C2E	C5-C6-N1	-3.03	119.17	123.48
2	E	201	C2E	C51-C61-N11	-3.02	119.19	123.48
2	J	201	C2E	O2A-C2A-C1A	-3.00	102.22	111.61
2	G	201	C2E	O21-P11-O5A	-2.97	94.11	108.14
2	H	201	C2E	C5-C6-N1	-2.96	119.26	123.48
2	E	201	C2E	C5-C6-N1	-2.95	119.29	123.48
2	F	201	C2E	C51-C61-N11	-2.93	119.31	123.48
2	D	202	C2E	C5-C6-N1	-2.92	119.32	123.48
2	J	201	C2E	O5'-C5'-C4'	-2.91	98.67	109.00
2	K	201	C2E	C5-C6-N1	-2.91	119.34	123.48
2	A	201	C2E	O6-C6-N1	-2.80	118.61	122.58
2	R	202	C2E	C41-C51-N71	-2.75	106.75	109.41
2	F	202	C2E	C41-C51-N71	-2.74	106.76	109.41
2	F	201	C2E	C1'-N9-C4	-2.71	121.95	126.64
2	R	202	C2E	O21-P11-O3'	-2.69	95.70	106.49
2	J	201	C2E	C6-C5-C4	-2.68	118.18	120.84
2	F	202	C2E	O21-P11-O3'	-2.67	95.74	106.49
2	F	201	C2E	C1A-N91-C41	-2.59	122.16	126.64
2	B	202	C2E	N21-C21-N11	-2.58	113.11	117.24
2	D	201	C2E	N21-C21-N11	-2.58	113.11	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	202	C2E	O2'-C2'-C3'	-2.58	103.84	111.18
2	E	202	C2E	O2'-C2'-C3'	-2.58	103.85	111.18
2	H	202	C2E	O2'-C2'-C3'	-2.58	103.85	111.18
2	B	202	C2E	O2'-C2'-C3'	-2.57	103.86	111.18
2	H	202	C2E	N21-C21-N11	-2.57	113.12	117.24
2	A	202	C2E	O2'-C2'-C3'	-2.57	103.87	111.18
2	N	202	C2E	O2'-C2'-C3'	-2.57	103.87	111.18
2	K	202	C2E	N21-C21-N11	-2.57	113.13	117.24
2	J	201	C2E	N3-C2-N1	-2.57	123.71	127.46
2	D	201	C2E	O2'-C2'-C3'	-2.56	103.89	111.18
2	G	202	C2E	N21-C21-N11	-2.56	113.15	117.24
2	G	202	C2E	O2'-C2'-C3'	-2.56	103.90	111.18
2	E	202	C2E	N21-C21-N11	-2.55	113.16	117.24
2	N	202	C2E	N21-C21-N11	-2.55	113.17	117.24
2	M	202	C2E	O2'-C2'-C3'	-2.55	103.94	111.18
2	A	202	C2E	N21-C21-N11	-2.55	113.17	117.24
2	M	202	C2E	N21-C21-N11	-2.54	113.18	117.24
2	G	202	C2E	N3-C2-N1	-2.53	123.76	127.46
2	F	201	C2E	C2A-C3A-C4A	-2.53	98.70	103.23
2	B	202	C2E	N3-C2-N1	-2.53	123.77	127.46
2	M	202	C2E	N3-C2-N1	-2.52	123.78	127.46
2	J	202	C2E	O2P-P1-O3A	-2.51	96.42	106.49
2	K	202	C2E	N3-C2-N1	-2.50	123.81	127.46
2	A	202	C2E	N3-C2-N1	-2.50	123.81	127.46
2	D	201	C2E	N3-C2-N1	-2.49	123.83	127.46
2	H	202	C2E	N3-C2-N1	-2.49	123.83	127.46
2	E	202	C2E	N3-C2-N1	-2.48	123.83	127.46
2	N	202	C2E	N3-C2-N1	-2.48	123.83	127.46
2	J	202	C2E	C2'-C3'-C4'	-2.47	98.80	103.23
2	B	201	C2E	O5'-C5'-C4'	-2.41	100.47	109.00
2	G	201	C2E	C2'-C3'-C4'	-2.33	99.07	103.23
2	F	202	C2E	C5-C6-N1	-2.32	120.17	123.48
2	J	202	C2E	C4'-O4'-C1'	-2.31	107.31	109.77
2	F	201	C2E	C5-C6-N1	-2.30	120.21	123.48
2	R	202	C2E	C5-C6-N1	-2.28	120.24	123.48
2	R	202	C2E	O2'-C2'-C1'	-2.25	104.57	111.61
2	F	202	C2E	O2'-C2'-C1'	-2.25	104.58	111.61
2	B	201	C2E	O21-P11-O3'	-2.12	97.99	106.49
2	E	201	C2E	N21-C21-N31	-2.04	113.98	117.75
2	D	202	C2E	N21-C21-N31	-2.03	114.00	117.75
2	H	202	C2E	O21-P11-O11	-2.03	101.78	112.28
2	B	202	C2E	O21-P11-O11	-2.03	101.78	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	C2E	C51-C61-N11	-2.03	120.60	123.48
2	M	202	C2E	O21-P11-O11	-2.03	101.79	112.28
2	K	202	C2E	O21-P11-O11	-2.03	101.80	112.28
2	E	202	C2E	O21-P11-O11	-2.02	101.80	112.28
2	N	202	C2E	O21-P11-O11	-2.02	101.80	112.28
2	K	201	C2E	N21-C21-N31	-2.02	114.01	117.75
2	G	202	C2E	O21-P11-O11	-2.02	101.81	112.28
2	A	202	C2E	O21-P11-O11	-2.02	101.82	112.28
2	D	201	C2E	O21-P11-O11	-2.02	101.83	112.28
2	A	201	C2E	N21-C21-N31	-2.02	114.02	117.75
2	G	202	C2E	C51-C61-N11	-2.02	120.61	123.48
2	H	201	C2E	N21-C21-N31	-2.01	114.03	117.75
2	E	202	C2E	C51-C61-N11	-2.01	120.63	123.48
2	B	201	C2E	C4-C5-N7	2.00	111.34	109.41
2	M	201	C2E	C41-C51-N71	2.01	111.35	109.41
2	J	201	C2E	C41-C51-N71	2.03	111.37	109.41
2	B	201	C2E	O21-P11-O11	2.03	122.79	112.28
2	G	201	C2E	O4A-C4A-C5A	2.06	116.34	109.40
2	R	202	C2E	C21-N31-C41	2.06	117.56	115.16
2	R	201	C2E	C3A-C2A-C1A	2.06	104.58	99.95
2	F	202	C2E	C21-N31-C41	2.07	117.58	115.16
2	J	202	C2E	O3'-C3'-C4'	2.12	118.00	110.04
2	B	201	C2E	N2-C2-N3	2.13	121.67	117.75
2	J	201	C2E	O4'-C4'-C5'	2.13	116.59	109.40
2	J	201	C2E	O3'-C3'-C2'	2.16	119.64	111.63
2	A	201	C2E	C5-C6-N1	2.19	119.26	115.75
2	B	201	C2E	C2-N3-C4	2.21	117.73	115.16
2	R	201	C2E	O3A-P1-O1P	2.23	118.23	109.46
2	G	201	C2E	C4-C5-N7	2.24	111.57	109.41
2	F	202	C2E	C2-N3-C4	2.26	117.80	115.16
2	R	202	C2E	C2-N3-C4	2.26	117.80	115.16
2	M	201	C2E	O3'-C3'-C4'	2.30	118.67	110.04
2	F	201	C2E	C5'-C4'-C3'	2.31	122.14	114.30
2	R	201	C2E	O21-P11-O11	2.32	124.30	112.28
2	R	201	C2E	C4'-O4'-C1'	2.33	112.25	109.77
2	J	201	C2E	C5'-C4'-C3'	2.43	122.53	114.30
2	R	201	C2E	C41-C51-N71	2.44	111.77	109.41
2	R	201	C2E	N2-C2-N1	2.44	121.15	117.24
2	R	201	C2E	O2P-P1-O1P	2.44	124.93	112.28
2	F	201	C2E	C5A-C4A-C3A	2.48	122.70	114.30
2	B	201	C2E	O4'-C4'-C5'	2.50	117.85	109.40
2	A	201	C2E	N21-C21-N11	2.51	121.25	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	C2E	N21-C21-N11	2.51	121.26	117.24
2	E	201	C2E	N21-C21-N11	2.52	121.27	117.24
2	D	202	C2E	N21-C21-N11	2.53	121.29	117.24
2	B	201	C2E	O2'-C2'-C1'	2.53	119.54	111.61
2	K	201	C2E	N21-C21-N11	2.54	121.30	117.24
2	N	201	C2E	C4A-O4A-C1A	2.55	112.48	109.77
2	M	201	C2E	O5'-P1-O1P	2.61	119.77	109.25
2	G	201	C2E	C3'-C2'-C1'	2.61	105.82	99.95
2	J	202	C2E	O2P-P1-O1P	2.61	125.81	112.28
2	R	201	C2E	N21-C21-N11	2.62	121.42	117.24
2	M	201	C2E	N2-C2-N1	2.63	121.45	117.24
2	N	201	C2E	C6-N1-C2	2.63	119.85	116.06
2	N	201	C2E	C4-C5-N7	2.64	111.96	109.41
2	R	201	C2E	O3'-P11-O11	2.65	119.90	109.46
2	B	201	C2E	C41-C51-N71	2.67	111.99	109.41
2	J	201	C2E	O4'-C4'-C3'	2.72	110.81	104.81
2	G	201	C2E	O21-P11-O11	2.72	126.38	112.28
2	N	201	C2E	C41-C51-N71	2.76	112.08	109.41
2	J	201	C2E	O2'-C2'-C1'	2.78	120.32	111.61
2	J	201	C2E	C3A-C2A-C1A	2.86	106.37	99.95
2	G	201	C2E	C1'-N9-C4	2.86	131.57	126.64
2	M	201	C2E	N21-C21-N11	2.86	121.82	117.24
2	J	202	C2E	C4-C5-N7	2.86	112.18	109.41
2	F	201	C2E	O4'-C4'-C3'	2.96	111.35	104.81
2	B	201	C2E	N21-C21-N11	2.99	122.02	117.24
2	E	201	C2E	C61-N11-C21	2.99	120.36	116.06
2	J	201	C2E	O3'-P11-O11	3.00	121.24	109.46
2	B	201	C2E	C5'-C4'-C3'	3.00	124.45	114.30
2	A	201	C2E	C61-N11-C21	3.01	120.38	116.06
2	R	202	C2E	C3'-C2'-C1'	3.02	106.72	99.95
2	J	201	C2E	C1'-N9-C4	3.02	131.85	126.64
2	H	201	C2E	C61-N11-C21	3.02	120.41	116.06
2	D	202	C2E	C61-N11-C21	3.03	120.42	116.06
2	F	202	C2E	C3'-C2'-C1'	3.04	106.78	99.95
2	K	201	C2E	C61-N11-C21	3.04	120.43	116.06
2	H	202	C2E	C2-N3-C4	3.24	118.94	115.16
2	E	202	C2E	C2-N3-C4	3.24	118.95	115.16
2	K	202	C2E	C2-N3-C4	3.25	118.96	115.16
2	D	201	C2E	C6-N1-C2	3.26	120.75	116.06
2	D	201	C2E	C2-N3-C4	3.27	118.97	115.16
2	M	202	C2E	C2-N3-C4	3.27	118.98	115.16
2	N	202	C2E	C2-N3-C4	3.27	118.98	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	C2E	O4'-C4'-C3'	3.27	112.03	104.81
2	A	202	C2E	C6-N1-C2	3.27	120.77	116.06
2	G	202	C2E	C2-N3-C4	3.28	118.99	115.16
2	J	202	C2E	C3'-C2'-C1'	3.28	107.32	99.95
2	F	201	C2E	C6-N1-C2	3.29	120.78	116.06
2	B	202	C2E	C2-N3-C4	3.29	119.00	115.16
2	E	202	C2E	C6-N1-C2	3.29	120.79	116.06
2	N	202	C2E	C6-N1-C2	3.29	120.79	116.06
2	A	202	C2E	C2-N3-C4	3.29	119.00	115.16
2	H	202	C2E	C6-N1-C2	3.29	120.80	116.06
2	J	202	C2E	N21-C21-N31	3.30	123.84	117.75
2	M	202	C2E	C6-N1-C2	3.31	120.81	116.06
2	K	202	C2E	C6-N1-C2	3.31	120.82	116.06
2	G	202	C2E	C6-N1-C2	3.32	120.83	116.06
2	B	202	C2E	C6-N1-C2	3.33	120.84	116.06
2	G	201	C2E	O2'-C2'-C3'	3.36	120.75	111.18
2	N	201	C2E	C3'-C2'-C1'	3.42	107.63	99.95
2	J	201	C2E	C1A-N91-C41	3.48	132.66	126.64
2	N	201	C2E	O21-P11-O11	3.55	130.64	112.28
2	M	201	C2E	C4-C5-N7	3.58	112.87	109.41
2	J	202	C2E	C6-N1-C2	3.59	121.23	116.06
2	N	201	C2E	C1A-N91-C41	3.79	133.19	126.64
2	B	201	C2E	C3'-C2'-C1'	3.82	108.54	99.95
2	J	201	C2E	O2'-C2'-C3'	3.89	122.25	111.18
2	R	201	C2E	C1'-N9-C4	3.89	133.36	126.64
2	N	201	C2E	O2'-C2'-C3'	3.91	122.29	111.18
2	G	201	C2E	C1A-N91-C41	3.91	133.39	126.64
2	M	201	C2E	C6-N1-C2	3.93	121.71	116.06
2	N	201	C2E	O2A-C2A-C3A	4.01	122.57	111.18
2	K	201	C2E	C6-N1-C2	4.04	121.87	116.06
2	H	201	C2E	C6-N1-C2	4.06	121.90	116.06
2	E	201	C2E	C6-N1-C2	4.07	121.91	116.06
2	D	202	C2E	C6-N1-C2	4.08	121.93	116.06
2	A	201	C2E	C8-N7-C5	4.09	111.32	103.35
2	M	201	C2E	O2'-C2'-C1'	4.10	124.43	111.61
2	B	201	C2E	C6-N1-C2	4.25	122.18	116.06
2	J	202	C2E	O2'-C2'-C1'	4.28	125.01	111.61
2	F	201	C2E	C61-N11-C21	4.35	122.32	116.06
2	B	201	C2E	C1'-N9-C4	4.39	134.23	126.64
2	J	202	C2E	O2'-C2'-C3'	4.41	123.71	111.18
2	J	201	C2E	C6-N1-C2	4.43	122.42	116.06
2	G	201	C2E	C6-N1-C2	4.43	122.42	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	201	C2E	C3'-C2'-C1'	4.45	109.94	99.95
2	F	201	C2E	O4A-C4A-C3A	4.46	114.64	104.81
2	K	201	C2E	O2'-C2'-C3'	4.51	124.01	111.18
2	A	201	C2E	O2'-C2'-C3'	4.51	124.02	111.18
2	D	202	C2E	O2'-C2'-C3'	4.52	124.02	111.18
2	H	201	C2E	O2'-C2'-C3'	4.52	124.03	111.18
2	E	201	C2E	C3'-C2'-C1'	4.54	110.15	99.95
2	E	201	C2E	O2'-C2'-C3'	4.54	124.09	111.18
2	R	201	C2E	C3'-C2'-C1'	4.54	110.16	99.95
2	A	201	C2E	C3'-C2'-C1'	4.55	110.18	99.95
2	D	202	C2E	C3'-C2'-C1'	4.56	110.20	99.95
2	N	201	C2E	C3A-C2A-C1A	4.57	110.21	99.95
2	H	201	C2E	C3'-C2'-C1'	4.57	110.21	99.95
2	K	201	C2E	C3'-C2'-C1'	4.57	110.21	99.95
2	M	201	C2E	C1A-N91-C41	4.57	134.53	126.64
2	R	201	C2E	C6-N1-C2	4.71	122.83	116.06
2	K	202	C2E	C2'-C3'-C4'	4.86	111.93	103.23
2	G	202	C2E	C2'-C3'-C4'	4.86	111.93	103.23
2	N	202	C2E	C2'-C3'-C4'	4.86	111.93	103.23
2	D	201	C2E	C2'-C3'-C4'	4.87	111.94	103.23
2	H	202	C2E	C2'-C3'-C4'	4.87	111.95	103.23
2	B	202	C2E	C2'-C3'-C4'	4.87	111.95	103.23
2	A	202	C2E	C2'-C3'-C4'	4.88	111.96	103.23
2	M	202	C2E	C2'-C3'-C4'	4.88	111.97	103.23
2	E	202	C2E	C2'-C3'-C4'	4.89	111.98	103.23
2	G	201	C2E	N21-C21-N11	5.12	125.42	117.24
2	R	201	C2E	C1A-N91-C41	5.14	135.52	126.64
2	D	201	C2E	O3'-C3'-C4'	5.30	129.94	110.04
2	A	202	C2E	O3'-C3'-C4'	5.31	129.97	110.04
2	M	202	C2E	O3'-C3'-C4'	5.31	129.97	110.04
2	E	202	C2E	O3'-C3'-C4'	5.31	129.98	110.04
2	B	202	C2E	O3'-C3'-C4'	5.31	129.98	110.04
2	N	202	C2E	O3'-C3'-C4'	5.31	129.98	110.04
2	G	202	C2E	O3'-C3'-C4'	5.32	130.00	110.04
2	K	202	C2E	O3'-C3'-C4'	5.32	130.01	110.04
2	H	202	C2E	O3'-C3'-C4'	5.32	130.01	110.04
2	R	201	C2E	O2'-C2'-C3'	5.45	126.67	111.18
2	B	201	C2E	C1A-N91-C41	5.73	136.53	126.64
2	B	201	C2E	O2'-C2'-C3'	5.96	128.14	111.18
2	J	202	C2E	C61-N11-C21	6.06	124.78	116.06
2	M	201	C2E	O2'-C2'-C3'	6.06	128.43	111.18
2	J	202	C2E	C1'-N9-C4	6.32	137.55	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	201	C2E	C61-N11-C21	6.35	125.19	116.06
2	J	202	C2E	C1A-N91-C41	6.47	137.82	126.64
2	J	201	C2E	C61-N11-C21	6.52	125.44	116.06
2	R	201	C2E	C61-N11-C21	6.83	125.89	116.06
2	B	201	C2E	C61-N11-C21	7.21	126.43	116.06
2	G	201	C2E	C61-N11-C21	7.48	126.83	116.06
2	N	201	C2E	C61-N11-C21	7.73	127.17	116.06
2	M	201	C2E	C1'-N9-C4	7.95	140.37	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	C2E	4	0
2	A	202	C2E	1	0
2	B	201	C2E	1	0
2	B	202	C2E	2	0
2	D	201	C2E	1	0
2	D	202	C2E	2	0
2	E	202	C2E	1	0
2	F	201	C2E	1	0
2	F	202	C2E	1	0
2	G	201	C2E	2	0
2	G	202	C2E	1	0
2	H	202	C2E	1	0
2	K	201	C2E	3	0
2	K	202	C2E	1	0
2	M	201	C2E	1	0
2	M	202	C2E	3	0
2	N	201	C2E	2	0
2	N	202	C2E	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	79/91 (86%)	0.63	5 (6%)	21 30	36, 50, 67, 74	0
1	B	72/91 (79%)	0.65	3 (4%)	37 47	31, 45, 71, 80	0
1	D	78/91 (85%)	0.66	6 (7%)	14 22	26, 43, 69, 72	0
1	E	75/91 (82%)	0.70	5 (6%)	19 28	32, 50, 74, 79	0
1	F	75/91 (82%)	0.52	1 (1%)	77 84	30, 45, 71, 78	0
1	G	75/91 (82%)	0.60	4 (5%)	27 37	27, 37, 65, 73	0
1	H	75/91 (82%)	0.64	3 (4%)	39 49	33, 49, 68, 74	0
1	J	78/91 (85%)	0.56	4 (5%)	29 39	25, 36, 68, 73	0
1	K	78/91 (85%)	0.48	2 (2%)	56 66	28, 40, 64, 67	0
1	M	75/91 (82%)	1.11	15 (20%)	1 1	33, 54, 87, 93	0
1	N	78/91 (85%)	0.51	3 (3%)	41 51	28, 40, 63, 70	0
1	R	78/91 (85%)	0.74	6 (7%)	14 22	24, 36, 71, 75	0
All	All	916/1092 (83%)	0.65	57 (6%)	21 31	24, 44, 72, 93	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ALA	7.9
1	J	160	ALA	7.7
1	R	161	VAL	7.4
1	R	160	ALA	6.1
1	M	155	ALA	5.1
1	E	83	PRO	4.9
1	M	158	ARG	4.7
1	M	91	ARG	4.6
1	D	161	VAL	4.6
1	M	157	ALA	4.5
1	D	160	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	M	156	ASP	4.1
1	A	161	VAL	3.9
1	R	159	ARG	3.7
1	H	152	VAL	3.6
1	R	155	ALA	3.5
1	J	159	ARG	3.4
1	N	160	ALA	3.4
1	K	129	LEU	3.4
1	M	83	PRO	3.4
1	G	157	ALA	3.2
1	M	119	GLY	3.2
1	R	130	ARG	3.0
1	E	155	ALA	2.9
1	G	155	ALA	2.9
1	E	85	LEU	2.9
1	A	84	LYS	2.9
1	B	95	VAL	2.9
1	H	156	ASP	2.8
1	M	93	ALA	2.7
1	G	83	PRO	2.7
1	D	159	ARG	2.6
1	E	157	ALA	2.6
1	A	82	PRO	2.6
1	M	95	VAL	2.6
1	M	154	ASP	2.6
1	E	158	ARG	2.5
1	R	157	ALA	2.5
1	D	95	VAL	2.5
1	B	98	GLU	2.5
1	J	155	ALA	2.4
1	D	90	GLU	2.3
1	N	159	ARG	2.3
1	M	122	LEU	2.3
1	B	154	ASP	2.3
1	D	158	ARG	2.2
1	H	83	PRO	2.1
1	M	84	LYS	2.1
1	M	96	PRO	2.1
1	N	161	VAL	2.1
1	J	156	ASP	2.1
1	G	158	ARG	2.1
1	F	85	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	89	LEU	2.0
1	M	153	LEU	2.0
1	A	156	ASP	2.0
1	K	160	ALA	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(Å ²)	Q<0.9
2	C2E	N	202	46/46	0.93	0.15	1.07	28,36,42,48	0
2	C2E	R	201	46/46	0.98	0.15	0.73	22,27,30,31	0
2	C2E	D	202	46/46	0.94	0.16	0.68	23,27,32,33	0
2	C2E	J	202	46/46	0.97	0.13	0.51	25,30,34,37	0
2	C2E	N	201	46/46	0.98	0.14	0.41	24,28,31,31	0
2	C2E	H	201	46/46	0.96	0.14	0.20	26,32,37,39	0
2	C2E	J	201	46/46	0.98	0.15	0.19	21,27,30,33	0
2	C2E	B	202	46/46	0.95	0.14	0.17	31,38,47,56	0
2	C2E	D	201	46/46	0.93	0.14	0.16	23,30,38,42	0
2	C2E	K	201	46/46	0.96	0.16	0.15	22,27,30,32	0
2	C2E	M	201	46/46	0.97	0.14	0.01	30,39,45,49	0
2	C2E	E	201	46/46	0.96	0.14	-0.01	27,34,37,39	0
2	C2E	F	201	46/46	0.94	0.14	-0.08	33,37,41,46	0
2	C2E	M	202	46/46	0.91	0.13	-0.09	40,49,55,61	0
2	C2E	F	202	46/46	0.93	0.13	-0.11	37,44,48,51	0
2	C2E	H	202	46/46	0.94	0.14	-0.18	33,40,51,53	0
2	C2E	G	201	46/46	0.98	0.14	-0.22	28,31,35,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	C2E	B	201	46/46	0.98	0.14	-0.30	25,33,38,40	0
2	C2E	A	201	45/46	0.95	0.13	-0.33	33,37,40,44	0
2	C2E	R	202	46/46	0.96	0.13	-0.40	27,32,41,44	0
2	C2E	K	202	46/46	0.96	0.12	-0.43	27,32,40,45	0
2	C2E	A	202	46/46	0.93	0.11	-0.55	39,46,52,59	0
2	C2E	E	202	46/46	0.94	0.12	-0.69	36,45,51,56	0
2	C2E	G	202	46/46	0.94	0.13	-0.78	31,40,52,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.