



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:46 PM GMT

PDB ID : 1H0M  
Title : THREE-DIMENSIONAL STRUCTURE OF THE QUORUM SENSING PROTEIN TRAR BOUND TO ITS AUTOINDUCER AND TO ITS TARGET DNA  
Authors : Vannini, A.; Volpari, C.; Gargioli, C.; Muraglia, E.; Cortese, R.; De Francesco, R.; Neddermann, P.; Di Marco, S.  
Deposited on : 2002-06-25  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

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

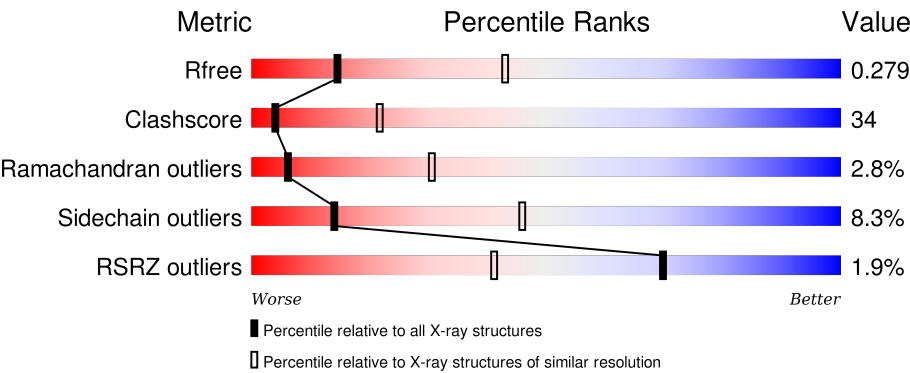
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



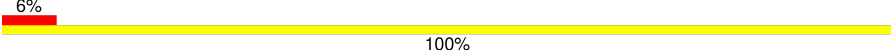
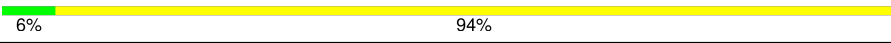
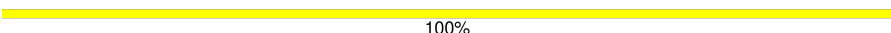
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	234	<div><div></div><div>58%32%7% ..</div></div>
1	B	234	<div><div></div><div>46%46%6% .</div></div>
1	C	234	<div><div>3%</div><div>57%35%5% ..</div></div>
1	D	234	<div><div>4%</div><div>43%48%6% .</div></div>
2	E	18	<div><div></div><div>11%89%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	18	 6% 100%
2	G	18	 6% 94%
2	H	18	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HSL	C	1235	-	-	-	X
4	OOA	C	1236	-	-	-	X
4	OOA	D	1236	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9013 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.

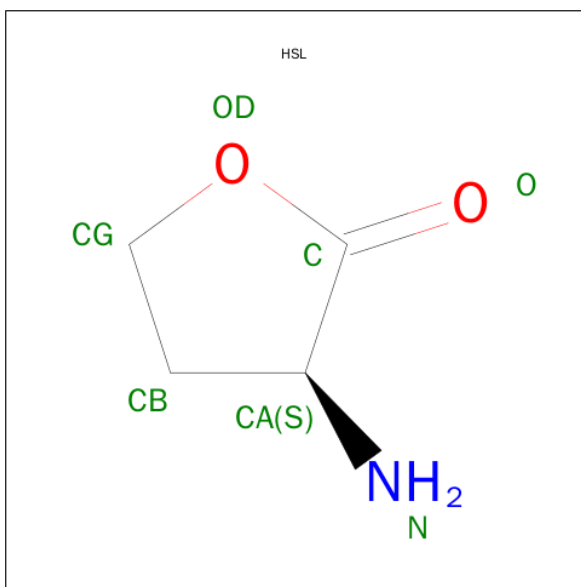
- Molecule 1 is a protein called TRANSCRIPTIONAL ACTIVATOR PROTEIN TRAR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	Se	0	0	0
			1859	1183	335	334	1	6			
1	B	230	Total	C	N	O	S	Se	0	0	0
			1851	1179	332	333	1	6			
1	C	228	Total	C	N	O	S	Se	0	0	0
			1844	1175	333	329	1	6			
1	D	229	Total	C	N	O	S	Se	0	0	0
			1843	1174	331	332	1	5			

- Molecule 2 is a DNA chain called 5'-D(\*AP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*AP\*TP \*CP\*TP\*GP\*CP\*AP\*CP\*AP\*T)-3'.

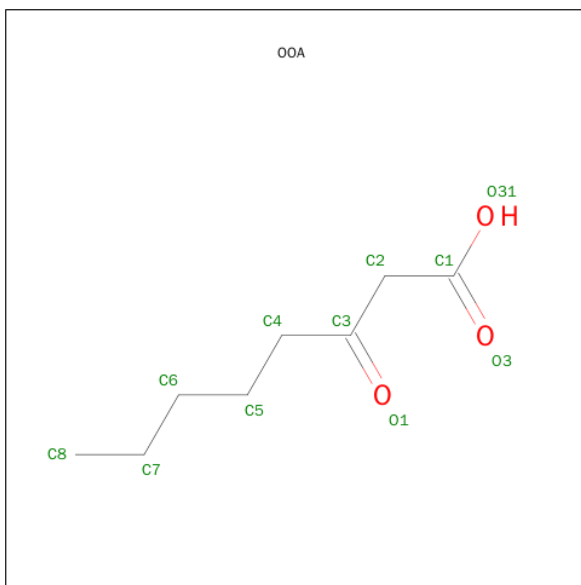
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			366	176	67	106	17			
2	F	18	Total	C	N	O	P	0	0	0
			366	176	67	106	17			
2	G	18	Total	C	N	O	P	0	0	0
			366	176	67	106	17			
2	H	18	Total	C	N	O	P	0	0	0
			366	176	67	106	17			

- Molecule 3 is HOMOSERINE LACTONE (three-letter code: HSL) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	4	1	2		
3	B	1	Total	C	N	O	0	0
			7	4	1	2		
3	C	1	Total	C	N	O	0	0
			7	4	1	2		
3	D	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 4 is 3-OXOOCTANOIC ACID (three-letter code: OOA) (formula: C<sub>8</sub>H<sub>14</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 8 2	0	0
4	B	1	Total C O 10 8 2	0	0
4	C	1	Total C O 10 8 2	0	0
4	D	1	Total C O 10 8 2	0	0

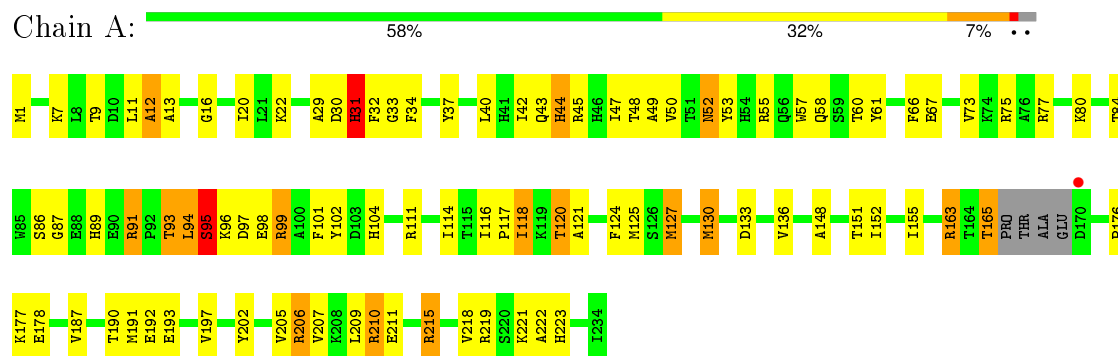
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	22	Total O 22 22	0	0
5	B	30	Total O 30 30	0	0
5	C	13	Total O 13 13	0	0
5	D	9	Total O 9 9	0	0
5	E	2	Total O 2 2	0	0
5	G	3	Total O 3 3	0	0
5	H	5	Total O 5 5	0	0

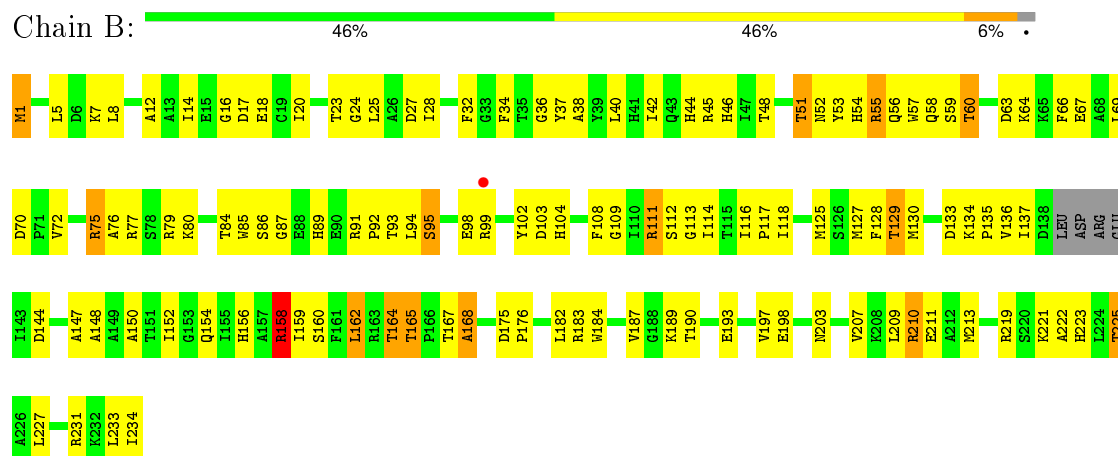
### 3 Residue-property plots

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

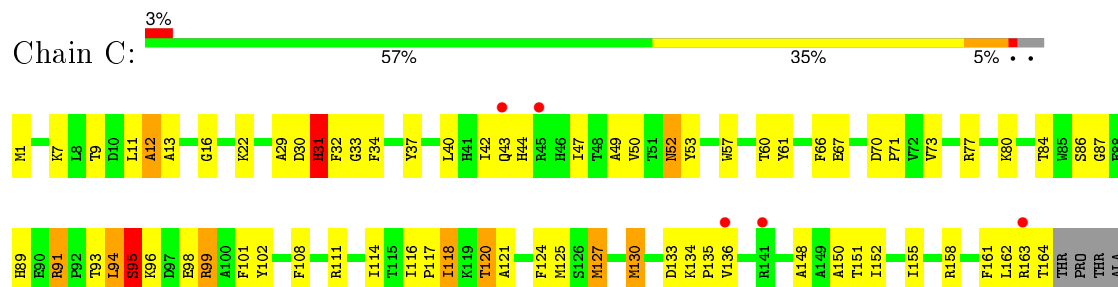
#### • Molecule 1: TRANSCRIPTIONAL ACTIVATOR PROTEIN TRAR



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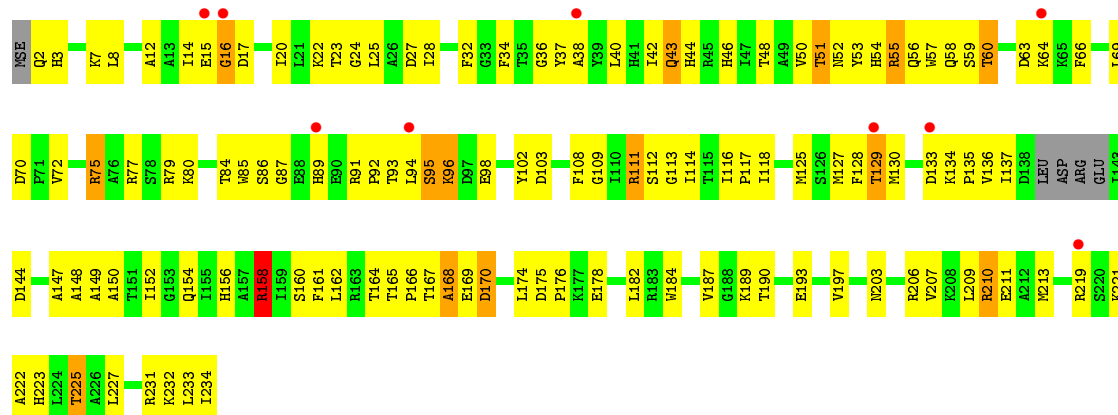
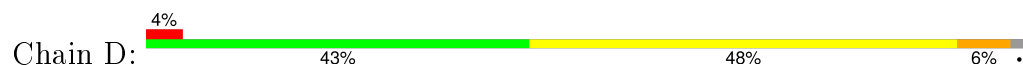


#### • Molecule 1: TRANSCRIPTIONAL ACTIVATOR PROTEIN TRAR

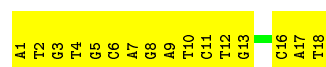
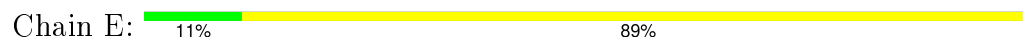




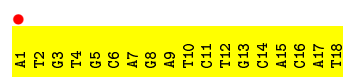
- Molecule 1: TRANSCRIPTIONAL ACTIVATOR PROTEIN TRAR



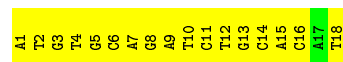
- Molecule 2: 5'-D(\*AP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*AP\*TP \*CP\*TP\*GP\*CP\*AP\*CP\*AP\*T)-3'



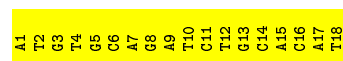
- Molecule 2: 5'-D(\*AP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*AP\*TP \*CP\*TP\*GP\*CP\*AP\*CP\*AP\*T)-3'



- Molecule 2: 5'-D(\*AP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*AP\*TP \*CP\*TP\*GP\*CP\*AP\*CP\*AP\*T)-3'



- Molecule 2: 5'-D(\*AP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*AP\*TP \*CP\*TP\*GP\*CP\*AP\*CP\*AP\*T)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.99 Å 94.68 Å 209.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-3.00) 97.4 (19.95-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.73 (at 2.98 Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, $R_{free}$	0.233 , 0.285 0.232 , 0.279	Depositor DCC
$R_{free}$ test set	1299 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 69.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 26681 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.48	0/1896	0.92	6/2549 (0.2%)
1	B	0.50	0/1889	1.13	10/2542 (0.4%)
1	C	0.43	0/1881	0.87	5/2528 (0.2%)
1	D	0.42	0/1881	1.11	9/2532 (0.4%)
2	E	0.48	0/410	0.77	0/631
2	F	0.46	0/410	0.80	0/631
2	G	0.46	0/410	0.77	0/631
2	H	0.43	0/410	0.78	0/631
All	All	0.46	0/9187	0.97	30/12675 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	ARG	NE-CZ-NH2	-18.40	111.10	120.30
1	D	219	ARG	NE-CZ-NH1	18.11	129.35	120.30
1	D	219	ARG	NE-CZ-NH2	-17.91	111.35	120.30
1	B	219	ARG	NE-CZ-NH1	-17.19	111.71	120.30
1	C	91	ARG	NE-CZ-NH1	17.01	128.81	120.30
1	D	55	ARG	NE-CZ-NH1	-16.83	111.88	120.30
1	D	158	ARG	NE-CZ-NH1	-16.75	111.93	120.30
1	B	219	ARG	NE-CZ-NH2	16.74	128.67	120.30
1	C	91	ARG	NE-CZ-NH2	-16.68	111.96	120.30
1	A	91	ARG	NE-CZ-NH2	16.65	128.62	120.30
1	D	55	ARG	NE-CZ-NH2	16.53	128.56	120.30
1	A	91	ARG	NE-CZ-NH1	-16.43	112.08	120.30
1	B	55	ARG	NE-CZ-NH2	-16.41	112.09	120.30
1	B	55	ARG	NE-CZ-NH1	16.37	128.49	120.30
1	B	158	ARG	NE-CZ-NH1	15.97	128.28	120.30
1	D	158	ARG	NE-CZ-NH2	15.79	128.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	SER	CB-CA-C	-13.08	85.24	110.10
1	D	219	ARG	CD-NE-CZ	10.26	137.96	123.60
1	B	219	ARG	CD-NE-CZ	9.66	137.13	123.60
1	A	91	ARG	CD-NE-CZ	9.44	136.81	123.60
1	C	91	ARG	CD-NE-CZ	9.39	136.74	123.60
1	D	55	ARG	CD-NE-CZ	9.31	136.64	123.60
1	B	55	ARG	CD-NE-CZ	9.17	136.43	123.60
1	A	96	LYS	N-CA-CB	-8.99	94.41	110.60
1	D	158	ARG	CD-NE-CZ	8.88	136.03	123.60
1	C	95	SER	CB-CA-C	-8.87	93.24	110.10
1	B	158	ARG	CD-NE-CZ	8.60	135.64	123.60
1	C	94	LEU	CB-CA-C	-6.31	98.20	110.20
1	B	162	LEU	CA-CB-CG	-5.22	103.30	115.30
1	A	97	ASP	N-CA-C	-5.11	97.22	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1859	0	1854	107	0
1	B	1851	0	1845	121	0
1	C	1844	0	1843	106	0
1	D	1843	0	1833	131	0
2	E	366	0	205	52	0
2	F	366	0	205	29	0
2	G	366	0	205	42	0
2	H	366	0	205	22	0
3	A	7	0	5	0	0
3	B	7	0	5	2	0
3	C	7	0	5	2	0
3	D	7	0	5	2	0
4	A	10	0	13	2	0
4	B	10	0	13	4	0
4	C	10	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	10	0	13	6	0
5	A	22	0	0	3	0
5	B	30	0	0	8	0
5	C	13	0	0	0	0
5	D	9	0	0	0	0
5	E	2	0	0	0	0
5	G	3	0	0	0	0
5	H	5	0	0	1	0
All	All	9013	0	8267	582	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 34.

All (582) 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:D:162:LEU:HD13	1:D:162:LEU:O	1.35	1.22
2:G:9:DA:H2''	2:G:10:DT:C5'	1.72	1.20
2:G:9:DA:H2''	2:G:10:DT:H5'	1.32	1.11
1:B:77:ARG:HA	1:B:125:MSE:HE1	1.27	1.11
2:H:14:DC:H2''	2:H:15:DA:H5'	1.33	1.10
1:D:77:ARG:HA	1:D:125:MSE:HE1	1.28	1.09
1:C:77:ARG:HA	1:C:125:MSE:HE1	1.35	1.09
2:G:11:DC:H2'	2:G:12:DT:H72	1.38	1.03
1:D:53:TYR:CD2	4:D:1236:OOA:H6C2	1.93	1.03
2:E:11:DC:H2''	2:E:12:DT:H5'	1.38	1.03
2:E:9:DA:H2''	2:E:10:DT:H5'	1.39	1.03
1:A:77:ARG:HA	1:A:125:MSE:HE1	1.41	1.03
1:C:1:MSE:HB3	1:C:199:GLY:HA3	1.38	1.02
1:C:73:VAL:HG22	1:C:127:MSE:HE1	1.41	1.00
1:A:73:VAL:HG22	1:A:127:MSE:HE1	1.43	0.97
1:C:1:MSE:SE	1:C:31:HIS:CD2	2.67	0.96
1:C:43:GLN:HG3	1:C:44:HIS:H	1.30	0.95
2:G:9:DA:H2''	2:G:10:DT:H5''	1.45	0.95
2:G:5:DG:H2''	2:G:6:DC:H5''	1.49	0.94
1:D:95:SER:HA	1:D:98:GLU:HB2	1.53	0.90
1:C:1:MSE:HB3	1:C:199:GLY:CA	2.01	0.90
2:G:4:DT:H2''	2:G:5:DG:H5'	1.53	0.90
1:C:91:ARG:HH11	1:C:99:ARG:HH12	1.13	0.89
2:G:11:DC:H2''	2:G:12:DT:H5'	1.56	0.88
1:C:61:TYR:HA	1:C:66:PHE:HD1	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:11:DC:H2'	2:G:12:DT:C7	2.04	0.88
2:E:4:DT:H2''	2:E:5:DG:H5'	1.55	0.87
1:A:40:LEU:HD12	1:A:127:MSE:CE	2.06	0.86
1:A:61:TYR:HA	1:A:66:PHE:HD1	1.38	0.86
1:D:162:LEU:CD1	1:D:162:LEU:O	2.21	0.86
2:H:5:DG:H2''	2:H:6:DC:H5''	1.54	0.85
1:A:215:ARG:HH11	1:A:215:ARG:CG	1.89	0.85
1:B:95:SER:HA	1:B:98:GLU:HB2	1.59	0.84
1:A:215:ARG:HH11	1:A:215:ARG:CB	1.91	0.84
2:E:9:DA:H2''	2:E:10:DT:C5'	2.08	0.84
1:C:91:ARG:HD3	1:C:99:ARG:NH1	1.93	0.83
1:D:158:ARG:NH1	1:D:162:LEU:HG	1.93	0.83
1:B:7:LYS:NZ	5:B:2003:HOH:O	2.03	0.83
1:C:94:LEU:O	1:C:94:LEU:HG	1.78	0.83
1:B:87:GLY:HA2	1:B:102:TYR:CE1	2.13	0.82
1:D:12:ALA:O	1:D:158:ARG:HG3	1.80	0.82
2:G:9:DA:C2'	2:G:10:DT:H5''	2.09	0.82
1:D:87:GLY:HA2	1:D:102:TYR:CE1	2.14	0.82
1:C:40:LEU:HD12	1:C:127:MSE:CE	2.10	0.81
1:D:22:LYS:NZ	1:D:167:THR:HG22	1.95	0.81
2:G:9:DA:C2'	2:G:10:DT:C5'	2.58	0.81
2:E:8:DG:H2''	2:E:9:DA:C5'	2.11	0.81
2:E:3:DG:H2''	2:E:4:DT:H5'	1.64	0.80
1:D:37:TYR:CE2	1:D:52:ASN:HB2	2.16	0.80
1:B:37:TYR:CE2	1:B:52:ASN:HB2	2.17	0.80
1:B:116:ILE:HD13	1:B:148:ALA:HB1	1.62	0.79
2:E:2:DT:H2''	2:E:3:DG:H5''	1.65	0.79
1:B:75:ARG:HH12	1:B:79:ARG:HH21	1.28	0.79
2:G:5:DG:C2'	2:G:6:DC:H5''	2.13	0.79
2:E:2:DT:C2'	2:E:3:DG:H5''	2.13	0.79
1:A:91:ARG:HE	1:A:99:ARG:NH1	1.81	0.78
1:C:43:GLN:HG3	1:C:44:HIS:N	1.97	0.78
1:D:42:ILE:HD11	1:D:127:MSE:CE	2.13	0.78
2:G:8:DG:H2''	2:G:9:DA:O5'	1.83	0.78
1:A:42:ILE:HG22	1:A:47:ILE:HG12	1.66	0.78
1:D:116:ILE:HD13	1:D:148:ALA:HB1	1.64	0.78
1:D:75:ARG:HH12	1:D:79:ARG:HH21	1.28	0.78
1:A:20:ILE:HG23	1:A:176:PRO:HD3	1.65	0.78
1:B:42:ILE:HD11	1:B:127:MSE:CE	2.13	0.78
1:C:42:ILE:HG22	1:C:47:ILE:HG12	1.66	0.77
1:D:53:TYR:HD2	4:D:1236:OOA:H6C2	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:H	1:B:221:LYS:NZ	1.83	0.77
2:F:2:DT:H2"	2:F:3:DG:C8	2.20	0.76
2:H:2:DT:H2"	2:H:3:DG:H5'	1.68	0.76
1:D:162:LEU:HD12	1:D:164:THR:HG23	1.67	0.76
2:F:14:DC:H2"	2:F:15:DA:H5'	1.67	0.76
2:H:5:DG:C2'	2:H:6:DC:H5"	2.17	0.75
2:E:8:DG:H2"	2:E:9:DA:H5'	1.69	0.75
2:F:1:DA:HO5'	2:F:1:DA:H8	1.33	0.75
1:A:219:ARG:HG3	2:E:13:DG:OP1	1.87	0.75
1:B:87:GLY:HA2	1:B:102:TYR:CD1	2.21	0.75
1:B:99:ARG:NH2	5:B:2019:HOH:O	2.19	0.75
2:E:18:DT:N3	2:F:1:DA:C2	2.52	0.74
2:G:2:DT:H1'	2:G:3:DG:H5"	1.66	0.74
1:C:95:SER:HB2	1:C:99:ARG:HB2	1.68	0.74
1:D:87:GLY:HA2	1:D:102:TYR:CD1	2.23	0.74
2:H:6:DC:H2"	2:H:7:DA:C8	2.22	0.74
1:C:207:VAL:O	1:C:210:ARG:HG3	1.88	0.74
1:C:221:LYS:HG2	2:G:12:DT:OP1	1.87	0.74
1:D:96:LYS:HD2	1:D:96:LYS:H	1.54	0.73
1:A:1:MSE:SE	1:A:31:HIS:HD2	2.20	0.73
1:D:56:GLN:O	1:D:60:THR:HG23	1.89	0.73
2:G:11:DC:H2"	2:G:12:DT:C5'	2.18	0.72
1:A:95:SER:HB3	1:A:99:ARG:HB2	1.70	0.72
1:A:207:VAL:O	1:A:210:ARG:HG3	1.90	0.72
1:B:17:ASP:HB3	1:B:20:ILE:HD12	1.69	0.72
1:A:215:ARG:NH1	1:A:215:ARG:HG3	2.04	0.72
1:D:221:LYS:HB3	5:H:2003:HOH:O	1.88	0.71
1:B:56:GLN:O	1:B:60:THR:HG23	1.91	0.71
1:A:12:ALA:HB2	1:A:155:ILE:HD13	1.72	0.71
1:A:61:TYR:HA	1:A:66:PHE:CD1	2.25	0.71
1:B:198:GLU:OE1	5:B:2028:HOH:O	2.08	0.71
1:C:222:ALA:H	1:D:221:LYS:NZ	1.87	0.71
1:A:118:ILE:HD12	1:B:150:ALA:HB1	1.73	0.71
1:B:93:THR:HG22	1:B:94:LEU:H	1.55	0.70
1:D:93:THR:HG22	1:D:94:LEU:H	1.55	0.70
2:G:3:DG:H2"	2:G:4:DT:C5'	2.21	0.70
2:G:3:DG:H2"	2:G:4:DT:H5"	1.73	0.70
1:D:53:TYR:CE2	4:D:1236:OOA:H2C1	2.27	0.70
1:C:1:MSE:SE	1:C:31:HIS:HD2	2.25	0.69
1:A:1:MSE:SE	1:A:31:HIS:CD2	2.96	0.69
1:C:219:ARG:HG3	2:G:13:DG:OP1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:VAL:O	1:C:187:VAL:HG12	1.92	0.69
2:F:17:DA:H2'	2:F:18:DT:H72	1.75	0.69
1:B:134:LYS:NZ	5:B:2021:HOH:O	2.25	0.69
2:G:15:DA:H2''	2:G:16:DC:H5'	1.75	0.69
1:B:38:ALA:HA	1:B:51:THR:HG23	1.74	0.68
2:E:2:DT:H2''	2:E:3:DG:C5'	2.22	0.68
1:C:118:ILE:HD12	1:D:150:ALA:HB1	1.75	0.68
2:H:8:DG:H2''	2:H:9:DA:OP2	1.94	0.68
2:F:4:DT:H2''	2:F:5:DG:H5'	1.75	0.68
2:F:5:DG:H1'	2:F:6:DC:H5'	1.76	0.68
2:F:5:DG:H2''	2:F:6:DC:H5'	1.75	0.68
1:D:162:LEU:HD12	1:D:164:THR:CG2	2.23	0.68
2:E:8:DG:H2''	2:E:9:DA:H5''	1.76	0.68
2:F:12:DT:H2''	2:F:13:DG:OP2	1.94	0.68
1:A:13:ALA:O	5:A:2003:HOH:O	2.11	0.68
2:H:12:DT:H1'	2:H:13:DG:H5'	1.74	0.67
3:B:1235:HSL:O	4:B:1236:OOA:H2C1	1.93	0.67
1:B:17:ASP:HB3	1:B:20:ILE:CD1	2.25	0.67
1:A:1:MSE:HE3	1:A:32:PHE:CE2	2.28	0.67
1:B:221:LYS:O	1:B:225:THR:HG23	1.94	0.67
1:C:163:ARG:HG2	1:C:164:THR:N	2.10	0.67
1:D:38:ALA:HA	1:D:51:THR:HG23	1.76	0.66
1:D:221:LYS:O	1:D:225:THR:HG23	1.95	0.66
1:D:66:PHE:HD2	1:D:69:LEU:HD12	1.59	0.66
1:A:215:ARG:NH1	1:A:215:ARG:CG	2.49	0.66
2:E:18:DT:H3	2:F:1:DA:H2	1.39	0.66
1:D:17:ASP:HB3	1:D:20:ILE:HD12	1.77	0.66
2:E:2:DT:H1'	2:E:3:DG:H5''	1.78	0.66
1:B:95:SER:HB3	5:B:2018:HOH:O	1.95	0.66
1:B:53:TYR:HE2	4:B:1236:OOA:H2C2	1.60	0.66
1:C:86:SER:HB2	1:C:136:VAL:HG12	1.76	0.66
1:B:159:ILE:O	1:B:164:THR:CG2	2.44	0.66
1:B:12:ALA:O	1:B:158:ARG:HG3	1.96	0.66
2:E:17:DA:H2''	2:E:18:DT:H73	1.78	0.65
1:B:53:TYR:CE2	4:B:1236:OOA:H2C2	2.31	0.65
1:C:1:MSE:HE3	1:C:32:PHE:CE2	2.32	0.65
1:B:45:ARG:HG3	1:B:45:ARG:HH11	1.62	0.65
1:C:61:TYR:HA	1:C:66:PHE:CD1	2.25	0.65
1:A:187:VAL:O	1:A:187:VAL:HG12	1.97	0.65
1:C:1:MSE:SE	1:C:31:HIS:NE2	2.80	0.65
1:B:89:HIS:O	1:B:92:PRO:HD2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LYS:HZ3	1:D:167:THR:HG22	1.62	0.65
1:A:91:ARG:HE	1:A:99:ARG:HH12	1.43	0.64
1:B:117:PRO:O	1:B:118:ILE:HD12	1.97	0.64
2:E:18:DT:C4	2:F:1:DA:N1	2.66	0.64
1:C:191:MSE:HG2	1:C:205:VAL:HG12	1.79	0.64
1:A:86:SER:HB2	1:A:136:VAL:HG12	1.79	0.64
1:C:77:ARG:CA	1:C:125:MSE:HE1	2.22	0.64
1:A:40:LEU:HD12	1:A:127:MSE:HE3	1.80	0.64
1:A:215:ARG:NE	5:A:2021:HOH:O	2.31	0.64
2:F:2:DT:H2''	2:F:3:DG:H8	1.60	0.64
1:C:12:ALA:HB2	1:C:155:ILE:HD13	1.80	0.64
1:A:120:THR:HG22	1:A:124:PHE:C	2.17	0.64
1:D:89:HIS:O	1:D:92:PRO:HD2	1.98	0.64
1:C:101:PHE:CE2	3:C:1235:HSL:HG2	2.33	0.63
1:B:77:ARG:CA	1:B:125:MSE:HE1	2.18	0.63
1:B:75:ARG:NH1	1:B:79:ARG:HH21	1.96	0.63
2:H:17:DA:H2'	2:H:18:DT:H72	1.81	0.63
1:B:116:ILE:HG21	1:B:152:ILE:HG13	1.79	0.63
1:B:40:LEU:HD11	4:B:1236:OOA:H4C1	1.81	0.63
1:A:191:MSE:HE3	1:A:209:LEU:HD12	1.80	0.63
1:C:191:MSE:CE	1:C:206:ARG:HA	2.29	0.63
1:B:175:ASP:HB2	1:B:176:PRO:HD2	1.81	0.63
1:D:37:TYR:CD2	1:D:52:ASN:HB2	2.34	0.63
2:G:5:DG:H2''	2:G:6:DC:C5'	2.26	0.63
2:E:3:DG:H2'	2:E:4:DT:C7	2.29	0.62
2:E:3:DG:H2'	2:E:4:DT:H72	1.80	0.62
2:F:5:DG:C2'	2:F:6:DC:H5'	2.30	0.62
1:D:17:ASP:HB3	1:D:20:ILE:CD1	2.30	0.62
1:D:158:ARG:HH11	1:D:162:LEU:HG	1.61	0.62
2:E:9:DA:H1'	2:E:10:DT:H5''	1.81	0.62
1:B:37:TYR:O	1:B:51:THR:HG22	2.00	0.62
1:D:117:PRO:O	1:D:118:ILE:HD12	2.00	0.61
1:D:116:ILE:HG21	1:D:152:ILE:HG13	1.83	0.61
1:A:91:ARG:HH11	1:A:99:ARG:HH12	1.48	0.61
1:D:85:TRP:CH2	3:D:1235:HSL:HB3	2.36	0.61
1:D:53:TYR:CE2	4:D:1236:OOA:H6C2	2.34	0.61
1:B:116:ILE:CD1	1:B:148:ALA:HB1	2.30	0.61
1:C:207:VAL:O	1:C:211:GLU:HG3	2.00	0.61
2:G:7:DA:C2	2:H:13:DG:N2	2.69	0.61
1:C:91:ARG:HD3	1:C:99:ARG:CZ	2.31	0.61
1:B:37:TYR:CD2	1:B:52:ASN:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASP:HB2	1:D:176:PRO:HD2	1.83	0.60
1:D:22:LYS:HZ2	1:D:167:THR:HG22	1.66	0.60
1:B:24:GLY:O	1:B:28:ILE:HG13	2.01	0.60
1:D:77:ARG:CA	1:D:125:MSE:HE1	2.19	0.60
2:E:17:DA:N9	2:E:18:DT:H72	2.17	0.60
1:C:118:ILE:HD12	1:D:150:ALA:CB	2.31	0.60
1:D:75:ARG:NH1	1:D:79:ARG:HH21	1.98	0.60
1:C:191:MSE:HE3	1:C:209:LEU:HD12	1.83	0.60
1:B:158:ARG:O	1:B:158:ARG:HD3	2.02	0.60
2:H:1:DA:H8	2:H:1:DA:HO5'	1.49	0.60
2:G:15:DA:H2''	2:G:16:DC:C5'	2.30	0.60
1:A:7:LYS:HD2	1:A:32:PHE:CE1	2.37	0.60
1:A:191:MSE:HG2	1:A:205:VAL:HG12	1.82	0.60
2:E:4:DT:C2'	2:E:5:DG:H5'	2.30	0.60
1:C:99:ARG:HD3	1:C:99:ARG:C	2.22	0.60
1:D:182:LEU:HD11	1:D:225:THR:HG22	1.82	0.59
1:B:150:ALA:O	1:B:154:GLN:HG3	2.01	0.59
1:D:24:GLY:O	1:D:28:ILE:HG13	2.03	0.59
2:E:9:DA:C2'	2:E:10:DT:C5'	2.80	0.59
1:D:116:ILE:CD1	1:D:148:ALA:HB1	2.32	0.59
1:D:167:THR:O	1:D:168:ALA:HB2	2.02	0.59
2:G:15:DA:H1'	2:G:16:DC:H5''	1.83	0.59
1:A:99:ARG:HD3	1:A:99:ARG:C	2.22	0.59
1:C:86:SER:OG	1:C:89:HIS:HB3	2.03	0.59
1:A:86:SER:OG	1:A:89:HIS:HB3	2.02	0.59
1:B:1:MSE:N	5:B:2001:HOH:O	2.34	0.59
1:D:150:ALA:O	1:D:154:GLN:HG3	2.03	0.59
1:C:120:THR:HG22	1:C:124:PHE:C	2.23	0.59
1:C:7:LYS:HD2	1:C:32:PHE:CE1	2.37	0.59
1:C:222:ALA:H	1:D:221:LYS:HZ3	1.49	0.59
1:B:44:HIS:ND1	5:B:2011:HOH:O	2.24	0.59
1:A:58:GLN:HA	4:A:1236:OOA:H8C3	1.85	0.59
1:B:95:SER:CA	1:B:98:GLU:HB2	2.29	0.58
1:C:9:THR:OG1	1:C:151:THR:HG22	2.04	0.58
1:D:53:TYR:HE2	4:D:1236:OOA:H2C1	1.69	0.58
1:A:215:ARG:HH11	1:A:215:ARG:HB2	1.66	0.58
2:E:2:DT:C1'	2:E:3:DG:H5''	2.32	0.58
1:B:57:TRP:HA	1:B:57:TRP:CE3	2.39	0.58
1:A:118:ILE:HD12	1:B:150:ALA:CB	2.33	0.58
1:D:85:TRP:CZ3	3:D:1235:HSL:HB3	2.38	0.58
1:A:207:VAL:O	1:A:211:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:SER:CA	1:D:98:GLU:HB2	2.28	0.58
1:B:187:VAL:HG12	1:B:187:VAL:O	2.04	0.58
1:C:40:LEU:HD12	1:C:127:MSE:HE3	1.85	0.58
1:B:64:LYS:HB3	1:B:66:PHE:CE2	2.39	0.58
2:E:18:DT:O4	2:F:1:DA:N1	2.36	0.58
1:A:1:MSE:HE3	1:A:32:PHE:CZ	2.39	0.58
1:B:75:ARG:HH12	1:B:79:ARG:NH2	2.00	0.57
2:G:9:DA:C2'	2:G:10:DT:H5'	2.22	0.57
2:G:3:DG:C8	2:G:4:DT:H72	2.39	0.57
1:C:202:TYR:CZ	1:C:206:ARG:HG3	2.39	0.57
1:D:162:LEU:HD13	1:D:162:LEU:C	2.19	0.57
2:F:12:DT:H1'	2:F:13:DG:H5'	1.87	0.57
1:B:182:LEU:HD11	1:B:225:THR:HG22	1.86	0.57
1:C:80:LYS:HA	1:C:117:PRO:HG2	1.87	0.57
2:E:1:DA:H2	2:F:18:DT:O2	1.88	0.57
2:E:11:DC:C2'	2:E:12:DT:H5'	2.24	0.56
1:A:84:THR:HG22	1:A:114:ILE:HG12	1.87	0.56
2:H:17:DA:H2'	2:H:18:DT:C7	2.35	0.56
1:D:37:TYR:O	1:D:51:THR:HG22	2.05	0.56
1:D:57:TRP:HA	1:D:57:TRP:CE3	2.40	0.56
1:D:187:VAL:O	1:D:187:VAL:HG12	2.05	0.56
1:C:116:ILE:HD13	1:C:148:ALA:HB1	1.88	0.56
1:C:187:VAL:CG1	1:C:187:VAL:O	2.54	0.56
1:D:66:PHE:CD2	1:D:69:LEU:HD12	2.38	0.56
1:C:193:GLU:O	1:C:197:VAL:HG23	2.06	0.56
2:E:3:DG:C8	2:E:4:DT:H72	2.40	0.56
2:H:3:DG:H1'	2:H:4:DT:H5''	1.88	0.56
1:A:43:GLN:O	1:A:44:HIS:HB2	2.06	0.56
1:A:191:MSE:CE	1:A:206:ARG:HA	2.36	0.56
1:D:64:LYS:HB3	1:D:66:PHE:CE2	2.41	0.56
1:D:23:THR:HG22	1:D:27:ASP:OD2	2.06	0.55
1:A:80:LYS:HA	1:A:117:PRO:HG2	1.88	0.55
2:F:17:DA:H2''	2:F:18:DT:O5'	2.06	0.55
1:C:84:THR:HG22	1:C:114:ILE:HG12	1.89	0.55
1:D:59:SER:O	1:D:63:ASP:OD2	2.25	0.55
1:B:59:SER:O	1:B:63:ASP:OD2	2.24	0.55
2:E:17:DA:N3	2:E:18:DT:C6	2.74	0.55
1:D:190:THR:OG1	1:D:193:GLU:HG3	2.07	0.55
2:F:17:DA:H2'	2:F:18:DT:C7	2.37	0.55
1:A:202:TYR:CZ	1:A:206:ARG:HG3	2.41	0.55
1:A:9:THR:OG1	1:A:151:THR:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:HD3	1:C:50:VAL:HG13	1.89	0.55
1:B:45:ARG:NH1	1:B:45:ARG:HG3	2.21	0.55
2:H:14:DC:H2''	2:H:15:DA:C5'	2.24	0.55
1:A:87:GLY:HA2	1:A:102:TYR:CE2	2.42	0.55
1:B:144:ASP:HB3	1:B:147:ALA:HB3	1.89	0.55
1:A:222:ALA:H	1:B:221:LYS:HZ3	1.53	0.54
1:B:159:ILE:O	1:B:164:THR:HG23	2.07	0.54
1:B:42:ILE:HD11	1:B:127:MSE:HE3	1.89	0.54
1:D:42:ILE:HD11	1:D:127:MSE:HE3	1.89	0.54
2:G:14:DC:H2''	2:G:15:DA:H5'	1.90	0.54
1:C:1:MSE:HE1	1:C:31:HIS:HD2	1.73	0.54
1:C:95:SER:HA	1:C:98:GLU:OE1	2.08	0.54
1:B:111:ARG:HB3	1:B:134:LYS:O	2.08	0.54
1:A:37:TYR:H	1:A:52:ASN:HB2	1.70	0.54
1:C:91:ARG:NH1	1:C:99:ARG:HH12	1.93	0.54
1:B:221:LYS:HG3	1:B:222:ALA:N	2.23	0.54
1:B:167:THR:O	1:B:168:ALA:HB2	2.07	0.54
1:B:93:THR:HG22	1:B:94:LEU:N	2.21	0.54
2:G:1:DA:H8	2:G:1:DA:HO5'	1.56	0.54
1:D:169:GLU:HG3	1:D:169:GLU:O	2.07	0.54
2:E:5:DG:H1'	2:E:6:DC:H5''	1.89	0.53
1:A:95:SER:CB	1:A:99:ARG:HB2	2.38	0.53
1:D:111:ARG:HB3	1:D:134:LYS:O	2.08	0.53
1:B:184:TRP:CE3	1:B:189:LYS:HG3	2.42	0.53
2:E:17:DA:C8	2:E:18:DT:H72	2.43	0.53
2:F:5:DG:C1'	2:F:6:DC:H5'	2.39	0.53
1:D:184:TRP:CE3	1:D:189:LYS:HG3	2.44	0.53
1:B:190:THR:OG1	1:B:193:GLU:HG3	2.08	0.53
1:C:1:MSE:HE3	1:C:32:PHE:CZ	2.43	0.53
1:B:116:ILE:CG2	1:B:152:ILE:HG13	2.38	0.53
1:B:34:PHE:CD1	1:B:130:MSE:HE3	2.43	0.53
1:C:1:MSE:CB	1:C:199:GLY:HA3	2.26	0.53
1:A:22:LYS:HD3	1:A:50:VAL:HG13	1.89	0.53
1:D:93:THR:HG22	1:D:94:LEU:N	2.21	0.53
1:C:40:LEU:CD2	1:C:49:ALA:HB2	2.38	0.53
2:F:15:DA:H1'	2:F:16:DC:H5'	1.91	0.53
1:B:148:ALA:O	1:B:152:ILE:HG12	2.09	0.53
1:D:75:ARG:HH12	1:D:79:ARG:NH2	2.01	0.53
1:C:37:TYR:H	1:C:52:ASN:HB2	1.71	0.53
1:A:223:HIS:CD2	1:B:187:VAL:HA	2.44	0.53
1:C:87:GLY:HA2	1:C:102:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:THR:HG22	1:B:27:ASP:OD2	2.09	0.52
1:D:144:ASP:HB3	1:D:147:ALA:HB3	1.89	0.52
1:C:191:MSE:HE2	1:C:206:ARG:HA	1.91	0.52
2:F:8:DG:H2"	2:F:9:DA:OP2	2.09	0.52
1:C:163:ARG:HG2	1:C:164:THR:H	1.74	0.52
1:B:34:PHE:CE1	1:B:130:MSE:HE3	2.45	0.52
1:D:86:SER:OG	1:D:136:VAL:HG12	2.10	0.52
1:A:48:THR:HG21	1:A:163:ARG:NH1	2.25	0.52
1:D:42:ILE:HD11	1:D:127:MSE:HE2	1.89	0.52
1:B:158:ARG:C	1:B:158:ARG:HD3	2.30	0.52
1:D:221:LYS:HG3	1:D:222:ALA:N	2.25	0.52
2:H:10:DT:H1'	2:H:11:DC:H5'	1.92	0.52
1:A:193:GLU:O	1:A:197:VAL:HG23	2.09	0.52
2:E:17:DA:H2"	2:E:18:DT:OP2	2.09	0.52
2:G:10:DT:C2	2:G:11:DC:C5	2.98	0.51
1:D:96:LYS:HD2	1:D:98:GLU:HG3	1.92	0.51
1:D:34:PHE:CD1	1:D:130:MSE:HE3	2.45	0.51
1:A:40:LEU:CD2	1:A:49:ALA:HB2	2.41	0.51
1:D:210:ARG:HA	1:D:213:MSE:HE3	1.92	0.51
2:H:14:DC:C2'	2:H:15:DA:H5'	2.22	0.51
1:D:116:ILE:CG2	1:D:152:ILE:HG13	2.39	0.51
2:F:5:DG:H1'	2:F:6:DC:C5'	2.40	0.51
1:B:8:LEU:HD21	1:B:128:PHE:CE2	2.46	0.51
1:C:77:ARG:HG2	1:C:125:MSE:CE	2.41	0.51
2:E:2:DT:C2	2:E:3:DG:C8	2.99	0.51
1:B:57:TRP:HE3	1:B:57:TRP:HA	1.75	0.51
1:B:91:ARG:N	1:B:92:PRO:CD	2.74	0.51
1:D:91:ARG:N	1:D:92:PRO:CD	2.74	0.51
1:C:161:PHE:HD1	1:D:161:PHE:HD2	1.59	0.51
1:C:120:THR:HG23	1:C:121:ALA:N	2.26	0.51
1:A:222:ALA:HB2	1:B:221:LYS:HZ2	1.75	0.51
1:B:46:HIS:CD2	1:B:231:ARG:CZ	2.93	0.51
1:D:77:ARG:HA	1:D:125:MSE:CE	2.20	0.50
1:D:38:ALA:HB3	1:D:129:THR:HG23	1.93	0.50
1:B:38:ALA:HB3	1:B:129:THR:HG23	1.94	0.50
1:B:46:HIS:HD2	1:B:231:ARG:CZ	2.25	0.50
1:B:203:ASN:O	1:B:207:VAL:HG23	2.11	0.50
1:A:93:THR:HG23	1:A:94:LEU:HG	1.91	0.50
1:C:111:ARG:HD2	1:C:133:ASP:O	2.12	0.50
1:A:187:VAL:CG1	1:A:187:VAL:O	2.59	0.50
2:G:12:DT:H6	2:G:12:DT:H5'	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:DC:H2"	2:H:17:DA:O5'	2.11	0.50
1:C:94:LEU:O	1:C:94:LEU:CG	2.52	0.50
2:G:3:DG:H2"	2:G:4:DT:H5'	1.92	0.50
1:D:203:ASN:O	1:D:207:VAL:HG23	2.11	0.50
1:A:116:ILE:HD13	1:A:148:ALA:HB1	1.93	0.50
1:A:120:THR:HG23	1:A:121:ALA:N	2.27	0.49
1:B:42:ILE:HD11	1:B:127:MSE:HE2	1.93	0.49
1:C:42:ILE:HG22	1:C:47:ILE:CG1	2.39	0.49
1:D:57:TRP:HE3	1:D:57:TRP:HA	1.76	0.49
1:D:34:PHE:CE1	1:D:130:MSE:HE3	2.47	0.49
1:D:184:TRP:CZ2	1:D:197:VAL:HG11	2.47	0.49
1:B:67:GLU:HB2	5:B:2014:HOH:O	2.11	0.49
1:B:17:ASP:H	1:B:20:ILE:HD12	1.77	0.49
2:H:5:DG:H2"	2:H:6:DC:C5'	2.34	0.49
1:B:112:SER:OG	1:B:137:ILE:HG23	2.13	0.49
1:D:80:LYS:NZ	1:D:125:MSE:HE2	2.28	0.49
1:C:43:GLN:CG	1:C:44:HIS:H	2.15	0.49
1:D:8:LEU:HD21	1:D:128:PHE:CE2	2.47	0.49
2:E:11:DC:H2"	2:E:12:DT:C5'	2.27	0.49
2:G:2:DT:C1'	2:G:3:DG:H5"	2.37	0.49
1:A:206:ARG:O	1:A:210:ARG:HG2	2.13	0.49
1:D:84:THR:HG22	1:D:114:ILE:HG12	1.95	0.49
1:A:30:ASP:O	1:A:33:GLY:N	2.36	0.49
1:B:54:HIS:CE1	1:B:55:ARG:HG2	2.47	0.49
1:A:77:ARG:HG2	1:A:125:MSE:CE	2.43	0.49
2:H:13:DG:H2"	2:H:14:DC:O5'	2.13	0.48
1:C:202:TYR:CE2	1:C:206:ARG:HG3	2.48	0.48
2:E:3:DG:H2"	2:E:4:DT:C5'	2.39	0.48
1:A:12:ALA:HB2	1:A:155:ILE:CD1	2.42	0.48
1:A:120:THR:HG22	1:A:125:MSE:N	2.28	0.48
1:C:99:ARG:O	1:C:99:ARG:HD3	2.13	0.48
1:B:36:GLY:HA2	1:B:52:ASN:OD1	2.13	0.48
1:A:111:ARG:HD2	1:A:133:ASP:O	2.13	0.48
2:G:10:DT:H2"	2:G:11:DC:O5'	2.14	0.48
1:B:128:PHE:CB	1:B:152:ILE:HD12	2.42	0.48
1:A:42:ILE:HG22	1:A:47:ILE:CG1	2.40	0.48
1:D:128:PHE:CB	1:D:152:ILE:HD12	2.44	0.48
1:B:193:GLU:O	1:B:197:VAL:HG23	2.13	0.48
1:A:221:LYS:N	2:E:12:DT:OP1	2.43	0.48
1:D:96:LYS:CE	1:D:98:GLU:HG3	2.44	0.48
1:A:165:THR:HG21	1:B:162:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:O	1:C:210:ARG:HG2	2.12	0.48
1:B:134:LYS:HB3	1:B:135:PRO:HD2	1.96	0.48
1:C:1:MSE:CE	1:C:31:HIS:HD2	2.27	0.48
2:H:9:DA:H2''	2:H:10:DT:C5'	2.44	0.48
1:D:36:GLY:HA2	1:D:52:ASN:OD1	2.14	0.47
2:F:13:DG:H2''	2:F:14:DC:O5'	2.13	0.47
1:D:148:ALA:O	1:D:152:ILE:HG12	2.15	0.47
1:C:86:SER:CB	1:C:136:VAL:HG12	2.43	0.47
2:G:1:DA:O5'	2:G:1:DA:H8	1.98	0.47
2:G:10:DT:C2	2:G:11:DC:C6	3.02	0.47
1:C:221:LYS:NZ	2:G:12:DT:OP2	2.45	0.47
1:A:42:ILE:CG2	1:A:47:ILE:HG12	2.41	0.47
2:G:12:DT:C6	2:G:12:DT:H5'	2.49	0.47
1:C:80:LYS:HZ1	1:C:125:MSE:HE2	1.80	0.47
1:A:80:LYS:NZ	1:A:125:MSE:HE2	2.29	0.47
1:D:193:GLU:O	1:D:197:VAL:HG23	2.13	0.47
1:C:98:GLU:O	1:C:101:PHE:HB3	2.15	0.47
2:E:17:DA:C2'	2:E:18:DT:H73	2.44	0.47
3:C:1235:HSL:O	4:C:1236:OOA:H2C1	2.14	0.47
2:E:17:DA:C4	2:E:18:DT:C5	3.03	0.47
1:A:202:TYR:CE2	1:A:206:ARG:HG3	2.50	0.46
1:C:158:ARG:HH12	1:C:162:LEU:HD23	1.80	0.46
1:C:91:ARG:CD	1:C:99:ARG:CZ	2.93	0.46
1:A:99:ARG:HD3	1:A:99:ARG:O	2.14	0.46
1:D:17:ASP:H	1:D:20:ILE:HD12	1.80	0.46
1:B:159:ILE:O	1:B:164:THR:HG22	2.14	0.46
1:D:134:LYS:HB3	1:D:135:PRO:HD2	1.98	0.46
2:E:4:DT:H6	2:E:4:DT:H5'	1.80	0.46
1:B:190:THR:HG23	1:B:193:GLU:OE1	2.16	0.46
1:B:210:ARG:HA	1:B:213:MSE:HE3	1.97	0.46
1:C:80:LYS:NZ	1:C:125:MSE:HE2	2.31	0.46
1:A:98:GLU:O	1:A:101:PHE:HB3	2.15	0.46
2:H:3:DG:H2''	2:H:4:DT:H5'	1.98	0.46
1:A:191:MSE:HE2	1:A:206:ARG:HA	1.98	0.46
1:C:150:ALA:HB1	1:D:118:ILE:HG13	1.96	0.46
1:B:86:SER:OG	1:B:136:VAL:HG12	2.15	0.46
2:F:11:DC:C2'	2:F:12:DT:H72	2.46	0.46
1:B:80:LYS:NZ	1:B:125:MSE:HE2	2.31	0.46
1:D:174:LEU:HD22	1:D:178:GLU:HB2	1.97	0.46
1:C:208:LYS:HA	1:C:208:LYS:HD3	1.78	0.46
1:D:85:TRP:CZ2	1:D:113:GLY:HA3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:THR:HG23	1:D:193:GLU:OE1	2.16	0.45
1:D:112:SER:OG	1:D:137:ILE:HG23	2.15	0.45
1:A:221:LYS:HG2	2:E:12:DT:OP1	2.17	0.45
1:D:156:HIS:O	1:D:160:SER:HB3	2.16	0.45
1:A:29:ALA:O	1:A:34:PHE:HB2	2.15	0.45
2:G:2:DT:C2'	2:G:3:DG:H5''	2.45	0.45
1:B:77:ARG:HA	1:B:125:MSE:CE	2.20	0.45
1:B:183:ARG:HD3	1:C:108:PHE:HA	1.99	0.45
1:A:95:SER:HA	1:A:98:GLU:OE1	2.16	0.45
2:E:3:DG:N9	2:E:4:DT:H72	2.32	0.45
1:D:25:LEU:HB3	1:D:37:TYR:CZ	2.52	0.45
2:G:4:DT:C2'	2:G:5:DG:H5'	2.38	0.45
1:B:40:LEU:CD1	1:B:127:MSE:HE3	2.46	0.45
1:C:42:ILE:CG2	1:C:47:ILE:HG12	2.42	0.45
1:C:191:MSE:CE	1:C:209:LEU:HB2	2.47	0.45
1:B:184:TRP:CZ2	1:B:197:VAL:HG11	2.51	0.45
1:B:84:THR:HG22	1:B:114:ILE:HG12	1.99	0.45
1:B:109:GLY:O	1:B:133:ASP:HA	2.17	0.45
1:B:25:LEU:HB3	1:B:37:TYR:CZ	2.52	0.45
1:C:29:ALA:O	1:C:34:PHE:HB2	2.16	0.45
2:F:7:DA:C2	2:F:8:DG:C2	3.06	0.45
2:E:9:DA:C1'	2:E:10:DT:H5''	2.47	0.44
1:D:50:VAL:HA	1:D:167:THR:HG23	1.98	0.44
1:A:86:SER:O	1:A:111:ARG:O	2.35	0.44
1:D:174:LEU:HD22	1:D:178:GLU:CB	2.47	0.44
1:D:54:HIS:CE1	1:D:55:ARG:HG2	2.52	0.44
1:A:118:ILE:HA	1:A:118:ILE:HD13	1.70	0.44
1:A:77:ARG:CA	1:A:125:MSE:HE1	2.28	0.44
1:A:191:MSE:HG2	1:A:205:VAL:CG1	2.46	0.44
1:B:18:GLU:OE2	1:B:165:THR:HG23	2.17	0.44
1:D:165:THR:HG23	1:D:166:PRO:HD2	2.00	0.44
4:D:1236:OOA:H5C2	4:D:1236:OOA:H8C2	1.69	0.44
1:D:96:LYS:N	1:D:96:LYS:HD2	2.29	0.44
1:A:191:MSE:CE	1:A:209:LEU:HB2	2.48	0.44
1:C:150:ALA:HB2	1:D:149:ALA:HB1	1.98	0.44
1:A:48:THR:HG21	1:A:163:ARG:CZ	2.48	0.44
1:B:207:VAL:O	1:B:211:GLU:HB2	2.18	0.44
1:D:2:GLN:HB3	1:D:3:HIS:H	1.53	0.44
1:D:51:THR:HG22	1:D:53:TYR:H	1.83	0.44
2:E:17:DA:C4	2:E:18:DT:H72	2.53	0.44
1:A:52:ASN:HA	1:A:52:ASN:HD22	1.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:TRP:O	1:C:61:TYR:HB2	2.18	0.43
1:A:91:ARG:NE	1:A:99:ARG:NH1	2.58	0.43
1:C:191:MSE:HG2	1:C:205:VAL:CG1	2.45	0.43
2:E:1:DA:H2''	2:E:2:DT:H5'	2.01	0.43
1:A:57:TRP:O	1:A:61:TYR:HB2	2.18	0.43
1:C:190:THR:OG1	1:C:193:GLU:HG3	2.18	0.43
1:B:209:LEU:O	1:B:213:MSE:HG3	2.18	0.43
1:D:167:THR:O	1:D:168:ALA:CB	2.65	0.43
1:B:85:TRP:CZ3	3:B:1235:HSL:HB3	2.52	0.43
1:D:40:LEU:CD1	1:D:127:MSE:HE3	2.48	0.43
1:B:85:TRP:CZ2	1:B:113:GLY:HA3	2.53	0.43
1:A:116:ILE:HB	1:A:152:ILE:HG13	2.01	0.43
1:C:158:ARG:HH12	1:C:162:LEU:CD2	2.32	0.43
1:A:34:PHE:CD1	1:A:130:MSE:HG3	2.53	0.43
2:E:17:DA:C2'	2:E:18:DT:C7	2.96	0.43
1:D:169:GLU:O	1:D:170:ASP:C	2.56	0.43
1:C:120:THR:HG22	1:C:125:MSE:N	2.33	0.43
1:C:118:ILE:HD13	1:C:118:ILE:HA	1.73	0.43
1:A:53:TYR:CE2	4:A:1236:OOA:H2C1	2.54	0.43
1:B:70:ASP:OD1	1:B:72:VAL:HB	2.19	0.43
1:B:116:ILE:O	1:B:127:MSE:HA	2.19	0.43
1:A:222:ALA:HB2	1:B:221:LYS:NZ	2.33	0.43
1:C:7:LYS:HD2	1:C:32:PHE:CZ	2.54	0.43
1:D:209:LEU:O	1:D:213:MSE:HG3	2.19	0.43
1:D:207:VAL:O	1:D:211:GLU:HB2	2.19	0.43
2:E:3:DG:C2'	2:E:4:DT:C7	2.95	0.42
1:D:166:PRO:C	1:D:168:ALA:H	2.21	0.42
1:A:95:SER:HB3	1:A:99:ARG:H	1.84	0.42
1:C:86:SER:O	1:C:111:ARG:O	2.37	0.42
1:A:86:SER:CB	1:A:136:VAL:HG12	2.47	0.42
1:A:177:LYS:O	1:A:178:GLU:C	2.57	0.42
1:B:94:LEU:O	1:B:95:SER:HB3	2.20	0.42
1:B:17:ASP:CB	1:B:20:ILE:HD12	2.42	0.42
1:D:43:GLN:HB3	1:D:44:HIS:H	1.64	0.42
2:E:11:DC:H2'	2:E:12:DT:H72	2.01	0.42
2:E:7:DA:H2''	2:E:8:DG:O5'	2.19	0.42
1:C:30:ASP:O	1:C:33:GLY:N	2.38	0.42
2:E:16:DC:H2''	2:E:17:DA:OP2	2.20	0.42
1:D:234:ILE:HG13	1:D:234:ILE:O	2.19	0.42
1:B:234:ILE:HG13	1:B:234:ILE:OXT	2.19	0.42
2:E:9:DA:C2'	2:E:10:DT:H5''	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PHE:HB3	1:B:152:ILE:HD12	2.02	0.42
1:C:12:ALA:HB2	1:C:155:ILE:CD1	2.49	0.42
1:A:218:VAL:HB	1:A:223:HIS:ND1	2.34	0.42
2:F:9:DA:H2''	2:F:10:DT:C5'	2.50	0.42
1:A:7:LYS:HD2	1:A:32:PHE:HE1	1.82	0.42
1:D:227:LEU:O	1:D:231:ARG:HG3	2.19	0.42
1:D:109:GLY:O	1:D:133:ASP:HA	2.20	0.42
1:B:80:LYS:HZ1	1:B:125:MSE:HE2	1.84	0.42
1:A:11:LEU:C	1:A:13:ALA:H	2.23	0.42
1:D:190:THR:HG23	1:D:193:GLU:CD	2.40	0.42
1:B:233:LEU:O	1:B:234:ILE:CG2	2.68	0.42
1:C:116:ILE:HB	1:C:152:ILE:HG13	2.02	0.42
1:C:11:LEU:C	1:C:13:ALA:H	2.23	0.42
1:C:7:LYS:HD2	1:C:32:PHE:HE1	1.81	0.42
1:B:51:THR:HG22	1:B:52:ASN:H	1.84	0.42
1:B:227:LEU:O	1:B:231:ARG:HG3	2.20	0.42
1:C:40:LEU:HD23	1:C:49:ALA:CB	2.50	0.41
2:G:3:DG:C2'	2:G:4:DT:H5''	2.44	0.41
1:D:7:LYS:HD3	1:D:32:PHE:HE1	1.84	0.41
1:A:45:ARG:O	1:A:47:ILE:HG13	2.21	0.41
1:A:80:LYS:HZ1	1:A:125:MSE:HE2	1.85	0.41
1:A:20:ILE:CG2	1:A:176:PRO:HD3	2.42	0.41
1:C:77:ARG:HG2	1:C:125:MSE:HE3	2.02	0.41
2:E:8:DG:H2''	2:E:9:DA:H8	1.85	0.41
2:F:18:DT:H2'	2:F:18:DT:OP2	2.21	0.41
1:D:15:GLU:HA	1:D:16:GLY:HA2	1.82	0.41
2:H:15:DA:H2''	2:H:16:DC:OP2	2.21	0.41
1:A:77:ARG:HG2	1:A:125:MSE:HE1	2.03	0.41
2:F:14:DC:C2'	2:F:15:DA:H5'	2.45	0.41
1:D:162:LEU:CG	1:D:162:LEU:O	2.67	0.41
2:F:17:DA:H2''	2:F:18:DT:C6	2.56	0.41
1:B:28:ILE:O	1:B:32:PHE:HD1	2.03	0.41
1:A:53:TYR:N	1:A:53:TYR:CD1	2.88	0.41
1:D:203:ASN:OD1	1:D:206:ARG:NH2	2.51	0.41
1:D:128:PHE:HB3	1:D:152:ILE:HD12	2.03	0.41
1:B:56:GLN:HB3	1:B:108:PHE:CE2	2.55	0.41
1:C:152:ILE:HD13	1:C:152:ILE:HA	1.90	0.41
1:C:77:ARG:HG2	1:C:125:MSE:HE1	2.02	0.41
2:E:3:DG:C2'	2:E:4:DT:H72	2.48	0.41
1:B:51:THR:HG22	1:B:53:TYR:H	1.86	0.41
1:B:76:ALA:O	1:B:79:ARG:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:CB	1:B:221:LYS:NZ	2.84	0.41
1:D:56:GLN:HB3	1:D:108:PHE:CE2	2.56	0.41
1:C:134:LYS:HB3	1:C:135:PRO:HD2	2.03	0.41
1:D:70:ASP:OD1	1:D:72:VAL:HB	2.20	0.41
1:B:5:LEU:HA	1:B:5:LEU:HD23	1.95	0.41
2:G:12:DT:C2	2:G:13:DG:C5	3.09	0.41
1:D:37:TYR:CD1	1:D:37:TYR:C	2.94	0.41
1:A:7:LYS:HD2	1:A:32:PHE:CZ	2.55	0.41
1:D:56:GLN:O	1:D:57:TRP:C	2.59	0.41
1:C:222:ALA:HB2	1:D:221:LYS:NZ	2.35	0.41
1:B:156:HIS:O	1:B:160:SER:HB3	2.20	0.41
1:B:56:GLN:O	1:B:57:TRP:C	2.60	0.40
1:A:55:ARG:HA	1:A:55:ARG:HD2	1.96	0.40
1:C:70:ASP:HA	1:C:71:PRO:HD3	1.92	0.40
1:A:91:ARG:NH1	1:A:99:ARG:HH12	2.16	0.40
1:C:34:PHE:CD1	1:C:130:MSE:HG3	2.56	0.40
2:G:11:DC:H2"	2:G:12:DT:C6	2.57	0.40
1:D:96:LYS:HE3	1:D:98:GLU:HG3	2.03	0.40
2:G:18:DT:O2	2:H:1:DA:H2	2.05	0.40
1:D:233:LEU:O	1:D:234:ILE:CG2	2.70	0.40
1:D:51:THR:HG22	1:D:52:ASN:H	1.85	0.40
1:C:40:LEU:HD23	1:C:49:ALA:HB2	2.03	0.40
1:A:190:THR:OG1	1:A:193:GLU:HG3	2.22	0.40
1:A:75:ARG:NE	5:A:2007:HOH:O	2.28	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	226/234 (97%)	197 (87%)	24 (11%)	5 (2%)	<b>8</b> 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	226/234 (97%)	199 (88%)	22 (10%)	5 (2%)	8	38
1	C	224/234 (96%)	198 (88%)	18 (8%)	8 (4%)	4	24
1	D	225/234 (96%)	190 (84%)	28 (12%)	7 (3%)	5	28
All	All	901/936 (96%)	784 (87%)	92 (10%)	25 (3%)	6	30

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ALA
1	A	95	SER
1	B	95	SER
1	C	12	ALA
1	D	168	ALA
1	B	16	GLY
1	B	58	GLN
1	C	93	THR
1	C	96	LYS
1	D	16	GLY
1	D	58	GLN
1	D	170	ASP
1	A	16	GLY
1	A	31	HIS
1	D	95	SER
1	D	232	LYS
1	A	44	HIS
1	B	168	ALA
1	C	16	GLY
1	C	31	HIS
1	C	53	TYR
1	C	95	SER
1	D	14	ILE
1	B	14	ILE
1	C	176	PRO

### 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	192/189 (102%)	174 (91%)	18 (9%)	11	39
1	B	191/189 (101%)	175 (92%)	16 (8%)	14	45
1	C	190/189 (100%)	175 (92%)	15 (8%)	15	48
1	D	190/189 (100%)	176 (93%)	14 (7%)	17	52
All	All	763/756 (101%)	700 (92%)	63 (8%)	14	46

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	52	ASN
1	A	60	THR
1	A	67	GLU
1	A	93	THR
1	A	94	LEU
1	A	99	ARG
1	A	104	HIS
1	A	118	ILE
1	A	120	THR
1	A	127	MSE
1	A	130	MSE
1	A	163	ARG
1	A	165	THR
1	A	192	GLU
1	A	206	ARG
1	A	210	ARG
1	A	215	ARG
1	B	1	MSE
1	B	48	THR
1	B	51	THR
1	B	60	THR
1	B	69	LEU
1	B	75	ARG
1	B	103	ASP
1	B	104	HIS
1	B	111	ARG
1	B	129	THR
1	B	158	ARG
1	B	164	THR
1	B	165	THR

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Mol	Chain	Res	Type
1	B	210	ARG
1	B	223	HIS
1	B	225	THR
1	C	31	HIS
1	C	52	ASN
1	C	60	THR
1	C	67	GLU
1	C	95	SER
1	C	99	ARG
1	C	118	ILE
1	C	120	THR
1	C	127	MSE
1	C	130	MSE
1	C	192	GLU
1	C	196	ASP
1	C	206	ARG
1	C	210	ARG
1	C	215	ARG
1	D	43	GLN
1	D	46	HIS
1	D	48	THR
1	D	51	THR
1	D	60	THR
1	D	75	ARG
1	D	96	LYS
1	D	103	ASP
1	D	111	ARG
1	D	129	THR
1	D	158	ARG
1	D	210	ARG
1	D	223	HIS
1	D	225	THR

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

Mol	Chain	Res	Type
1	A	31	HIS
1	A	43	GLN
1	A	52	ASN
1	B	46	HIS
1	C	31	HIS
1	C	52	ASN

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Mol	Chain	Res	Type
1	D	104	HIS

### 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 ⓘ

8 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$
3	HSL	A	1235	4	6,7,7	3.42	2 (33%)	4,9,9	3.67	2 (50%)
4	OOA	A	1236	3	9,9,10	0.43	0	6,9,11	0.87	0
3	HSL	B	1235	4	6,7,7	3.40	2 (33%)	4,9,9	4.10	2 (50%)
4	OOA	B	1236	3	9,9,10	1.15	1 (11%)	6,9,11	0.92	0
3	HSL	C	1235	4	6,7,7	3.52	2 (33%)	4,9,9	3.35	2 (50%)
4	OOA	C	1236	3	9,9,10	0.54	0	6,9,11	0.90	0
3	HSL	D	1235	4	6,7,7	3.61	2 (33%)	4,9,9	3.83	2 (50%)
4	OOA	D	1236	3	9,9,10	0.53	0	6,9,11	0.89	0

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
3	HSL	A	1235	4	-	0/0/10/10	0/1/1/1
4	OOA	A	1236	3	-	0/7/8/9	0/0/0/0
3	HSL	B	1235	4	-	0/0/10/10	0/1/1/1
4	OOA	B	1236	3	-	0/7/8/9	0/0/0/0
3	HSL	C	1235	4	-	0/0/10/10	0/1/1/1
4	OOA	C	1236	3	-	0/7/8/9	0/0/0/0
3	HSL	D	1235	4	-	0/0/10/10	0/1/1/1
4	OOA	D	1236	3	-	0/7/8/9	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1236	OOA	C2-C3	-3.17	1.48	1.52
3	C	1235	HSL	OD-CG	2.94	1.53	1.46
3	A	1235	HSL	OD-CG	2.95	1.53	1.46
3	D	1235	HSL	OD-CG	2.97	1.53	1.46
3	B	1235	HSL	OD-CG	3.00	1.54	1.46
3	B	1235	HSL	OD-C	7.59	1.52	1.35
3	A	1235	HSL	OD-C	7.68	1.52	1.35
3	C	1235	HSL	OD-C	7.99	1.52	1.35
3	D	1235	HSL	OD-C	8.21	1.53	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1235	HSL	CG-OD-C	-5.64	105.48	110.62
3	D	1235	HSL	CG-OD-C	-4.95	106.11	110.62
3	A	1235	HSL	CG-OD-C	-4.60	106.43	110.62
3	C	1235	HSL	CG-OD-C	-4.38	106.63	110.62
3	C	1235	HSL	OD-C-O	4.99	126.95	121.44
3	A	1235	HSL	OD-C-O	5.66	127.69	121.44
3	D	1235	HSL	OD-C-O	5.83	127.88	121.44
3	B	1235	HSL	OD-C-O	5.88	127.93	121.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1236	OOA	2	0
3	B	1235	HSL	2	0
4	B	1236	OOA	4	0
3	C	1235	HSL	2	0
4	C	1236	OOA	1	0
3	D	1235	HSL	2	0
4	D	1236	OOA	6	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	224/234 (95%)	-0.42	1 (0%) 93 80	17, 49, 101, 150	0
1	B	224/234 (95%)	-0.40	1 (0%) 93 80	21, 51, 108, 145	0
1	C	222/234 (94%)	-0.20	6 (2%) 58 28	36, 68, 126, 159	0
1	D	224/234 (95%)	0.23	9 (4%) 42 17	33, 88, 145, 178	0
2	E	18/18 (100%)	0.29	0 100 100	50, 91, 141, 149	0
2	F	18/18 (100%)	0.33	1 (5%) 28 11	59, 84, 134, 165	0
2	G	18/18 (100%)	0.41	0 100 100	60, 99, 123, 130	0
2	H	18/18 (100%)	0.26	0 100 100	63, 93, 151, 153	0
All	All	966/1008 (95%)	-0.16	18 (1%) 70 41	17, 66, 130, 178	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	15	GLU	6.2
1	D	38	ALA	5.0
1	A	170	ASP	4.8
1	C	171	ALA	4.5
1	D	133	ASP	4.2
1	D	16	GLY	3.1
1	D	89	HIS	2.9
1	D	129	THR	2.9
1	D	94	LEU	2.6
1	D	64	LYS	2.5
1	C	163	ARG	2.5
1	B	99	ARG	2.5
1	C	141	ARG	2.2
1	D	219	ARG	2.2
2	F	1	DA	2.2
1	C	43	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	136	VAL	2.1
1	C	45	ARG	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	HSL	C	1235	7/7	0.93	0.39	5.90	65,65,65,65	0
4	OOA	C	1236	10/11	0.92	0.34	2.25	65,65,65,65	0
3	HSL	A	1235	7/7	0.91	0.29	1.72	44,44,44,44	0
3	HSL	D	1235	7/7	0.83	0.40	1.64	106,106,106,106	0
3	HSL	B	1235	7/7	0.99	0.25	1.60	45,45,45,45	0
4	OOA	D	1236	10/11	0.85	0.47	1.30	106,106,106,106	0
4	OOA	A	1236	10/11	0.90	0.28	0.97	44,44,44,44	0
4	OOA	B	1236	10/11	0.97	0.24	0.89	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.