



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 11:37 PM EDT

PDB ID : 1L3L
Title : Crystal structure of a bacterial quorum-sensing transcription factor complexed with pheromone and DNA
Authors : Zhang, R.; Pappas, T.; Brace, J.L.; Miller, P.C.; Oulmassov, T.; Molyneaux, J.M.; Anderson, J.C.; Bashkin, J.K.; Winans, S.C.; Joachimiak, A.
Deposited on : unknown
Resolution : 1.66 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

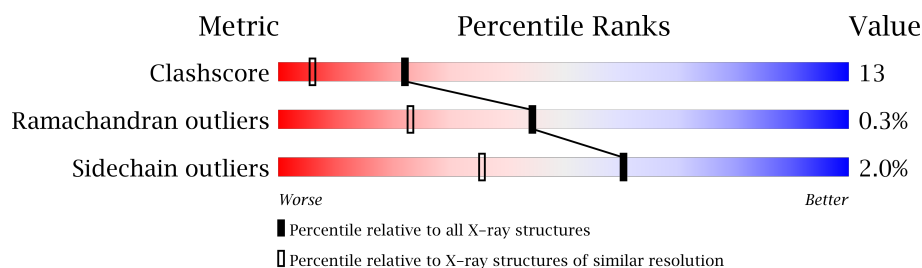
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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))
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	20	
1	F	20	
1	G	20	
1	H	20	
2	A	234	
2	B	234	
2	C	234	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	234	<div><div></div><div>71%</div><div>24%</div><div></div><div>.</div><div>.</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9942 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 DNA chain called 5'-D(*GP*AP*TP*GP*TP*GP*CP*AP*GP*AP*TP*C
P*TP*GP*CP*AP*CP*AP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	20	Total	C	N	O	P	0	0	0
			407	195	75	118	19			
1	F	20	Total	C	N	O	P	0	0	0
			407	195	75	118	19			
1	G	20	Total	C	N	O	P	0	0	0
			407	195	75	118	19			
1	H	20	Total	C	N	O	P	0	0	0
			407	195	75	118	19			

- Molecule 2 is a protein called Transcriptional activator protein traR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	233	Total	C	N	O	S	Se	0	0	0
			1847	1179	328	334	1	5			
2	B	233	Total	C	N	O	S	Se	0	0	0
			1843	1173	330	334	1	5			
2	C	225	Total	C	N	O	S	Se	0	0	0
			1821	1162	327	325	1	6			
2	D	225	Total	C	N	O	S	Se	0	0	0
			1821	1162	327	325	1	6			

There are 24 discrepancies between the modelled and reference sequences:

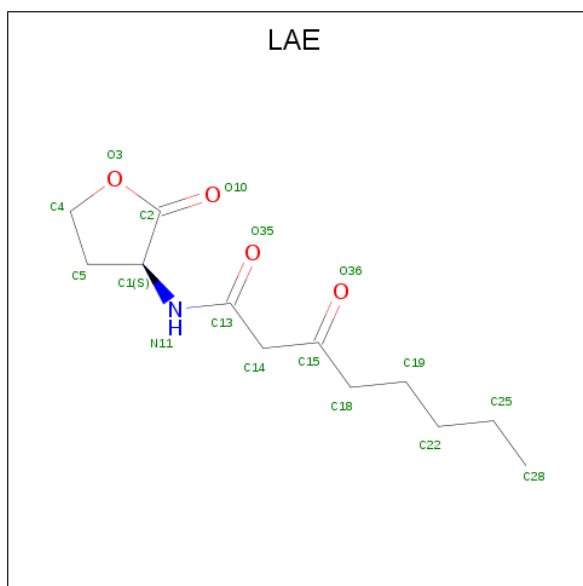
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P33905
A	125	MSE	MET	MODIFIED RESIDUE	UNP P33905
A	127	MSE	MET	MODIFIED RESIDUE	UNP P33905
A	130	MSE	MET	MODIFIED RESIDUE	UNP P33905
A	191	MSE	MET	MODIFIED RESIDUE	UNP P33905
A	213	MSE	MET	MODIFIED RESIDUE	UNP P33905
B	1	MSE	MET	MODIFIED RESIDUE	UNP P33905

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	125	MSE	MET	MODIFIED RESIDUE	UNP P33905
B	127	MSE	MET	MODIFIED RESIDUE	UNP P33905
B	130	MSE	MET	MODIFIED RESIDUE	UNP P33905
B	191	MSE	MET	MODIFIED RESIDUE	UNP P33905
B	213	MSE	MET	MODIFIED RESIDUE	UNP P33905
C	1	MSE	MET	MODIFIED RESIDUE	UNP P33905
C	125	MSE	MET	MODIFIED RESIDUE	UNP P33905
C	127	MSE	MET	MODIFIED RESIDUE	UNP P33905
C	130	MSE	MET	MODIFIED RESIDUE	UNP P33905
C	191	MSE	MET	MODIFIED RESIDUE	UNP P33905
C	213	MSE	MET	MODIFIED RESIDUE	UNP P33905
D	1	MSE	MET	MODIFIED RESIDUE	UNP P33905
D	125	MSE	MET	MODIFIED RESIDUE	UNP P33905
D	127	MSE	MET	MODIFIED RESIDUE	UNP P33905
D	130	MSE	MET	MODIFIED RESIDUE	UNP P33905
D	191	MSE	MET	MODIFIED RESIDUE	UNP P33905
D	213	MSE	MET	MODIFIED RESIDUE	UNP P33905

- Molecule 3 is 3-OXO-OCTANOIC ACID (2-OXO-TETRAHYDRO-FURAN-3-YL)-AMIDE (three-letter code: LAE) (formula: C₁₂H₁₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	12	1	4		
3	B	1	Total	C	N	O	0	0
			17	12	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			17	12	1	4		
3	D	1	Total	C	N	O	0	0
			17	12	1	4		

- Molecule 4 is water.

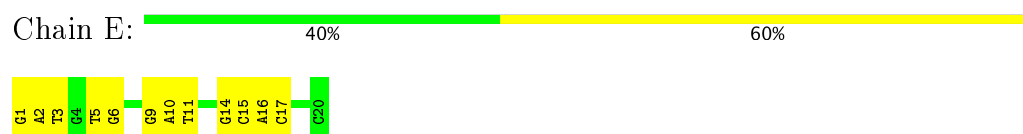
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	45	Total	O	0	0
			45	45		
4	F	41	Total	O	0	0
			41	41		
4	G	56	Total	O	0	0
			56	56		
4	H	51	Total	O	0	0
			51	51		
4	A	148	Total	O	0	0
			148	148		
4	B	161	Total	O	0	0
			161	161		
4	C	207	Total	O	0	0
			207	207		
4	D	205	Total	O	0	0
			205	205		

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.

Note EDS was not executed.

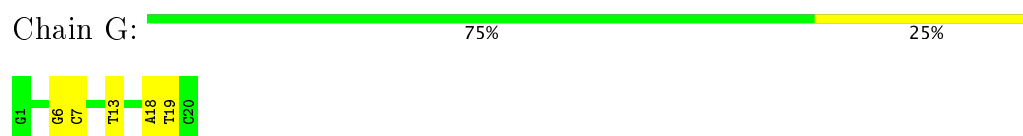
- Molecule 1: 5'-D(*GP*AP*TP*GP*TP*GP*CP*AP*GP*AP*TP*CP*TP*GP*CP*AP*CP*AP*TP*C)-3'



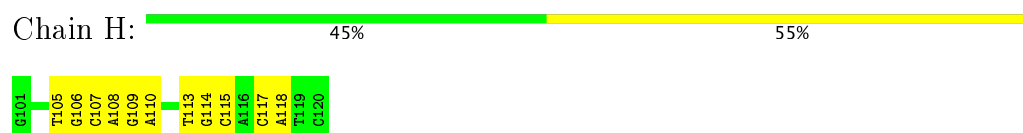
- Molecule 1: 5'-D(*GP*AP*TP*GP*TP*GP*CP*AP*GP*AP*TP*CP*TP*GP*CP*AP*CP*AP*TP*C)-3'



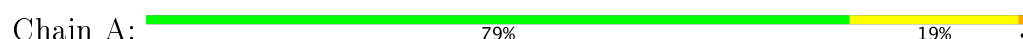
- Molecule 1: 5'-D(*GP*AP*TP*GP*TP*GP*CP*AP*GP*AP*TP*CP*TP*GP*CP*AP*CP*AP*TP*C)-3'

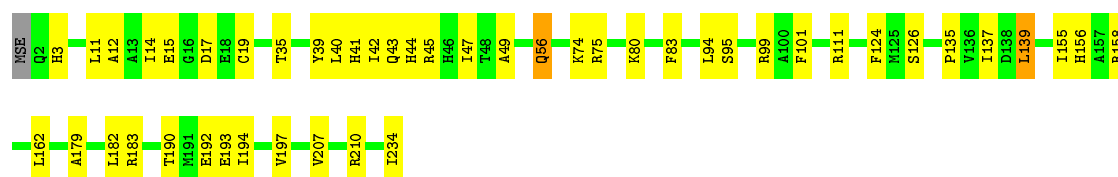


- Molecule 1: 5'-D(*GP*AP*TP*GP*TP*GP*CP*AP*GP*AP*TP*CP*TP*GP*CP*AP*CP*AP*TP*C)-3'



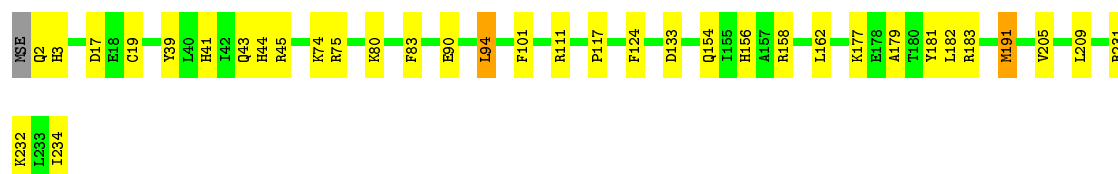
- Molecule 2: Transcriptional activator protein traR





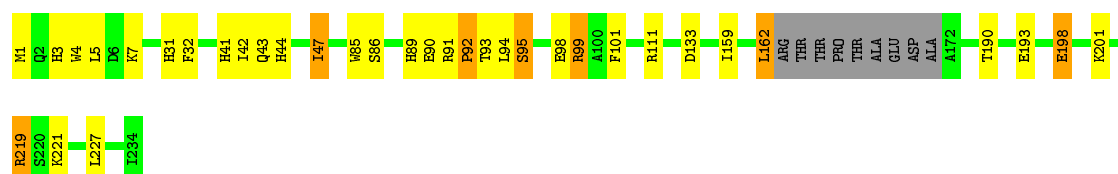
- Molecule 2: Transcriptional activator protein traR

Chain B: 85% 14%



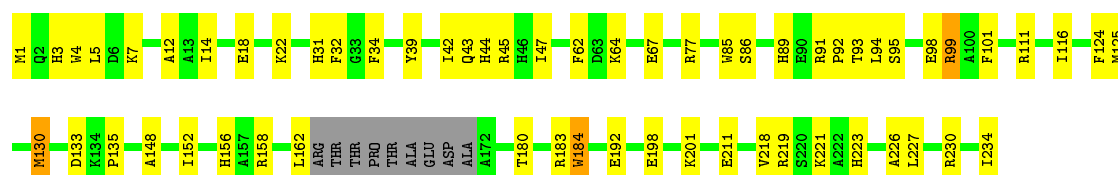
- Molecule 2: Transcriptional activator protein traR

Chain C: 81% 12%



- Molecule 2: Transcriptional activator protein traR

Chain D: 71% 24%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.30 Å 58.37 Å 127.45 Å 90.00° 102.81° 90.00°	Depositor
Resolution (Å)	39.60 – 1.66	Depositor
% Data completeness (in resolution range)	89.1 (39.60-1.66)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9942	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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: LAE

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	E	0.39	0/456	0.71	0/702
1	F	0.38	0/456	0.74	0/702
1	G	0.40	0/456	0.76	0/702
1	H	0.39	0/456	0.73	0/702
2	A	0.34	0/1886	0.59	0/2545
2	B	0.33	0/1882	0.60	0/2540
2	C	0.36	0/1858	0.59	0/2497
2	D	0.35	0/1858	0.60	0/2497
All	All	0.35	0/9308	0.63	0/12887

There are no bond length outliers.

There are no bond angle outliers.

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	E	407	0	227	18	0
1	F	407	0	227	9	0
1	G	407	0	227	4	0
1	H	407	0	227	12	0
2	A	1847	0	1816	52	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1843	0	1798	36	0
2	C	1821	0	1818	38	0
2	D	1821	0	1818	63	0
3	A	17	0	19	2	0
3	B	17	0	19	1	0
3	C	17	0	19	2	0
3	D	17	0	19	3	0
4	A	148	0	0	3	0
4	B	161	0	0	6	0
4	C	207	0	0	5	0
4	D	205	0	0	9	0
4	E	45	0	0	1	0
4	F	41	0	0	2	0
4	G	56	0	0	1	0
4	H	51	0	0	0	0
All	All	9942	0	8234	228	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 13.

All (228) 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)
2:D:77:ARG:HG2	2:D:125:MSE:HE1	1.25	1.15
1:H:106:DG:H2''	1:H:107:DC:H5''	1.59	0.84
1:E:10:DA:H2''	1:E:11:DT:H5'	1.60	0.83
1:E:5:DT:H2''	1:E:6:DG:H5'	1.63	0.80
2:A:183:ARG:HG2	2:A:234:ILE:HG23	1.64	0.79
2:D:226:ALA:O	2:D:230:ARG:HG2	1.84	0.78
2:B:183:ARG:HG2	2:B:234:ILE:HG23	1.66	0.77
2:D:91:ARG:HB3	2:D:92:PRO:HD3	1.67	0.77
2:D:1:MSE:HE1	2:D:31:HIS:HD2	1.51	0.76
1:E:2:DA:H2''	1:E:3:DT:H5'	1.68	0.75
1:G:6:DG:H2''	1:G:7:DC:H5'	1.68	0.75
1:E:10:DA:H2''	1:E:11:DT:C5'	2.16	0.75
1:F:110:DA:H2''	1:F:111:DT:H5'	1.70	0.74
1:F:110:DA:H2''	1:F:111:DT:C5'	2.17	0.74
2:D:34:PHE:CG	2:D:130:MSE:HG3	2.22	0.73
2:C:1:MSE:HE1	2:C:31:HIS:CD2	2.24	0.73
2:C:1:MSE:HE1	2:C:31:HIS:HD2	1.54	0.73
2:A:183:ARG:HG2	2:A:234:ILE:CG2	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MSE:HE2	2:D:32:PHE:CZ	2.24	0.72
2:B:234:ILE:HG22	2:B:234:ILE:OXT	1.90	0.71
1:E:2:DA:H1'	1:E:3:DT:H5''	1.72	0.70
1:F:105:DT:H2''	1:F:106:DG:H5'	1.74	0.70
2:D:184:TRP:HZ3	2:D:198:GLU:OE2	1.75	0.69
2:D:77:ARG:CG	2:D:125:MSE:HE1	2.14	0.69
4:E:537:HOH:O	2:D:201:LYS:HE2	1.93	0.68
1:H:107:DC:H2''	1:H:108:DA:C8	2.28	0.68
2:A:137:ILE:CG2	2:A:139:LEU:HD13	2.25	0.67
2:D:1:MSE:HE1	2:D:31:HIS:CD2	2.29	0.67
2:B:3:HIS:HA	4:B:1020:HOH:O	1.93	0.67
2:D:3:HIS:HE1	4:D:1089:HOH:O	1.77	0.67
2:B:205:VAL:O	2:B:209:LEU:HD23	1.95	0.66
1:H:106:DG:C2'	1:H:107:DC:H5''	2.25	0.66
2:B:177:LYS:HG3	4:B:1147:HOH:O	1.95	0.66
2:A:44:HIS:O	4:A:1026:HOH:O	2.12	0.66
2:D:44:HIS:HB2	4:D:1205:HOH:O	1.95	0.66
1:H:114:DG:H2''	1:H:115:DC:H5''	1.78	0.65
2:C:7:LYS:HE2	2:C:198:GLU:OE1	1.95	0.65
1:E:1:DG:H8	1:E:1:DG:HO5'	1.44	0.65
2:C:47:ILE:HD13	4:C:1071:HOH:O	1.95	0.65
2:B:44:HIS:O	4:B:1023:HOH:O	2.14	0.65
2:D:99:ARG:HH11	2:D:99:ARG:HG3	1.62	0.64
2:C:3:HIS:CD2	2:C:5:LEU:H	2.15	0.64
2:C:1:MSE:HE2	2:C:32:PHE:CZ	2.33	0.64
2:D:45:ARG:HD2	2:D:67:GLU:OE2	1.97	0.63
1:E:2:DA:H2''	1:E:3:DT:C5'	2.29	0.63
2:C:3:HIS:HD2	2:C:5:LEU:H	1.44	0.63
2:D:156:HIS:HE1	4:D:1185:HOH:O	1.80	0.63
4:F:133:HOH:O	2:A:192:GLU:HG3	1.98	0.63
2:D:91:ARG:HA	2:D:94:LEU:HD12	1.81	0.61
2:A:179:ALA:O	2:A:183:ARG:HG3	2.01	0.61
2:D:42:ILE:HG12	2:D:47:ILE:HG22	1.83	0.61
2:C:219:ARG:HD2	2:C:219:ARG:N	2.15	0.60
2:D:86:SER:HB3	2:D:89:HIS:HB3	1.83	0.60
2:B:2:GLN:HG2	2:B:3:HIS:CD2	2.36	0.60
2:D:3:HIS:CD2	2:D:5:LEU:H	2.19	0.60
2:C:41:HIS:CE1	2:C:43:GLN:HE21	2.20	0.60
2:D:34:PHE:CD2	2:D:130:MSE:HG3	2.37	0.60
1:E:16:DA:H2''	1:E:17:DC:H5'	1.83	0.59
2:C:198:GLU:HG2	4:C:1153:HOH:O	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:LYS:HZ1	2:D:198:GLU:HA	1.67	0.59
2:B:43:GLN:HG2	2:B:124:PHE:CD2	2.38	0.59
2:C:44:HIS:HB2	4:C:1171:HOH:O	2.03	0.58
1:G:18:DA:H2"	1:G:19:DT:H5'	1.85	0.58
2:D:184:TRP:CZ3	2:D:198:GLU:OE2	2.55	0.58
2:D:91:ARG:HD2	2:D:99:ARG:CZ	2.33	0.58
2:B:156:HIS:HE1	4:B:1059:HOH:O	1.86	0.58
2:A:56:GLN:HE21	2:A:56:GLN:HA	1.69	0.58
2:B:2:GLN:N	4:B:1060:HOH:O	2.35	0.58
2:C:3:HIS:HE1	4:C:1090:HOH:O	1.86	0.58
2:D:135:PRO:HD2	4:D:1069:HOH:O	2.03	0.58
2:D:116:ILE:HD13	2:D:148:ALA:HB1	1.87	0.57
2:D:3:HIS:HD2	2:D:5:LEU:H	1.51	0.57
1:E:14:DG:H2"	1:E:15:DC:H5'	1.87	0.57
2:A:74:LYS:NZ	2:A:74:LYS:HB2	2.20	0.57
2:D:218:VAL:HG12	2:D:223:HIS:CE1	2.40	0.57
2:A:42:ILE:HD12	2:A:47:ILE:HG12	1.87	0.56
2:C:86:SER:HB3	2:C:89:HIS:HB3	1.87	0.56
2:A:40:LEU:HD12	2:A:47:ILE:CG2	2.35	0.56
2:B:234:ILE:HG22	2:D:230:ARG:HH22	1.69	0.56
2:A:137:ILE:HG22	2:A:139:LEU:HD13	1.88	0.56
2:D:92:PRO:O	2:D:93:THR:OG1	2.21	0.56
2:A:40:LEU:HB3	2:A:42:ILE:HD11	1.87	0.55
2:B:39:TYR:OH	2:B:156:HIS:HD2	1.89	0.55
2:C:41:HIS:HE1	2:C:43:GLN:HE21	1.55	0.55
4:G:21:HOH:O	2:D:192:GLU:HG3	2.07	0.55
2:D:95:SER:OG	2:D:98:GLU:HG3	2.06	0.54
2:A:101:PHE:CE2	3:A:1003:LAE:H42	2.42	0.54
2:B:101:PHE:CE2	3:B:1001:LAE:H42	2.43	0.54
1:F:110:DA:H2"	1:F:111:DT:H5"	1.89	0.53
2:D:91:ARG:HG3	4:D:1159:HOH:O	2.07	0.53
2:A:15:GLU:OE1	2:A:162:LEU:HD11	2.08	0.53
1:E:16:DA:H1'	1:E:17:DC:H5"	1.91	0.52
2:D:99:ARG:HG3	2:D:99:ARG:NH1	2.24	0.52
2:C:91:ARG:HD3	4:C:1059:HOH:O	2.09	0.52
2:C:99:ARG:HH11	2:C:99:ARG:HG3	1.75	0.52
2:D:183:ARG:CZ	2:D:234:ILE:HG23	2.39	0.52
2:A:156:HIS:HE1	4:A:1058:HOH:O	1.92	0.51
2:B:181:TYR:CB	2:B:209:LEU:HD21	2.39	0.51
2:D:91:ARG:HD2	2:D:99:ARG:NH2	2.25	0.51
2:A:40:LEU:HD21	3:A:1003:LAE:H192	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:TYR:OH	2:A:156:HIS:HD2	1.94	0.51
1:H:114:DG:C2'	1:H:115:DC:H5''	2.41	0.51
2:B:74:LYS:HB2	2:B:74:LYS:NZ	2.26	0.50
2:C:159:ILE:O	2:C:162:LEU:HB2	2.11	0.50
2:A:194:ILE:O	2:A:197:VAL:HG12	2.12	0.50
1:F:110:DA:C2'	1:F:111:DT:H5''	2.41	0.50
1:F:109:DG:H2''	1:F:110:DA:OP2	2.11	0.50
2:C:227:LEU:HD23	2:C:227:LEU:C	2.32	0.50
2:D:39:TYR:OH	2:D:156:HIS:HD2	1.95	0.50
2:B:90:GLU:C	2:B:94:LEU:HD22	2.32	0.50
2:C:91:ARG:N	2:C:92:PRO:HD2	2.26	0.50
2:D:43:GLN:HA	2:D:124:PHE:CD1	2.46	0.50
1:H:109:DG:H2''	1:H:110:DA:OP2	2.11	0.50
2:A:75:ARG:HD3	2:A:83:PHE:CE2	2.47	0.50
2:D:91:ARG:O	2:D:94:LEU:HB2	2.11	0.50
2:A:14:ILE:HG23	2:A:14:ILE:O	2.12	0.49
2:B:43:GLN:HG2	2:B:124:PHE:CG	2.47	0.49
2:A:39:TYR:C	2:A:40:LEU:HD22	2.33	0.49
2:B:234:ILE:CG2	2:D:230:ARG:HH22	2.26	0.49
2:C:91:ARG:HD2	2:C:99:ARG:CZ	2.43	0.49
2:C:47:ILE:HD13	2:C:47:ILE:H	1.77	0.49
1:G:13:DT:OP2	2:D:221:LYS:NZ	2.44	0.49
2:A:95:SER:O	2:A:99:ARG:HG3	2.14	0.48
2:A:43:GLN:HG2	2:A:124:PHE:CD2	2.48	0.48
2:A:40:LEU:HD12	2:A:47:ILE:HG21	1.95	0.48
2:A:15:GLU:HA	2:A:15:GLU:OE2	2.13	0.48
1:H:105:DT:H2''	1:H:106:DG:O5'	2.14	0.48
2:B:44:HIS:O	2:B:45:ARG:HB2	2.13	0.48
2:A:40:LEU:CD1	2:A:49:ALA:HB2	2.42	0.48
2:D:45:ARG:HB2	4:D:1196:HOH:O	2.13	0.48
2:C:91:ARG:HA	2:C:94:LEU:HD12	1.94	0.48
2:D:14:ILE:HA	2:D:183:ARG:NH1	2.29	0.48
2:A:44:HIS:O	2:A:45:ARG:HB2	2.13	0.48
2:A:40:LEU:HD13	2:A:49:ALA:HB2	1.96	0.48
1:E:2:DA:C1'	1:E:3:DT:H5''	2.44	0.48
1:H:113:DT:OP2	2:C:221:LYS:NZ	2.45	0.48
2:C:101:PHE:CE2	3:C:1004:LAE:H42	2.49	0.47
2:D:91:ARG:HB3	2:D:92:PRO:CD	2.42	0.47
2:B:182:LEU:HG	2:B:234:ILE:HD11	1.95	0.47
2:D:219:ARG:HH11	2:D:219:ARG:HG2	1.78	0.47
2:B:181:TYR:HB2	2:B:209:LEU:HD21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:DA:C2'	1:E:3:DT:C5'	2.92	0.47
2:A:14:ILE:O	2:A:14:ILE:CG2	2.63	0.47
2:B:75:ARG:HD3	2:B:83:PHE:CE2	2.50	0.47
2:A:42:ILE:HD12	2:A:47:ILE:CG1	2.44	0.47
2:B:183:ARG:HG2	2:B:234:ILE:CG2	2.42	0.46
2:A:158:ARG:NH1	2:A:162:LEU:HD12	2.29	0.46
2:B:41:HIS:CD2	2:B:43:GLN:HE21	2.33	0.46
2:A:35:THR:HG22	2:A:35:THR:O	2.15	0.46
2:A:42:ILE:HD12	2:A:47:ILE:CD1	2.46	0.46
2:D:227:LEU:C	2:D:227:LEU:HD23	2.35	0.46
2:A:42:ILE:HG23	2:A:47:ILE:HG12	1.96	0.46
2:B:154:GLN:NE2	4:B:1138:HOH:O	2.49	0.46
2:A:42:ILE:HD13	2:A:47:ILE:HG23	1.98	0.45
2:B:158:ARG:HD2	2:B:162:LEU:HD12	1.97	0.45
2:A:182:LEU:CD2	2:A:234:ILE:HD11	2.45	0.45
2:C:7:LYS:HD3	2:C:32:PHE:HE2	1.81	0.45
1:E:9:DG:H2''	1:E:10:DA:OP2	2.16	0.45
1:E:10:DA:H2''	1:E:11:DT:H5''	1.98	0.44
1:H:107:DC:H5'	1:H:107:DC:H6	1.81	0.44
2:A:190:THR:OG1	2:A:193:GLU:HG3	2.17	0.44
2:B:179:ALA:O	2:B:183:ARG:HG3	2.18	0.44
2:D:180:THR:HG21	4:D:1082:HOH:O	2.16	0.44
1:E:10:DA:C2'	1:E:11:DT:C5'	2.93	0.44
2:D:12:ALA:O	2:D:158:ARG:HD3	2.17	0.44
2:D:219:ARG:NH1	2:D:219:ARG:HG2	2.31	0.44
2:A:41:HIS:CD2	2:A:43:GLN:HE21	2.35	0.44
1:E:2:DA:H1'	1:E:3:DT:C5'	2.45	0.44
2:A:42:ILE:CD1	2:A:47:ILE:HG23	2.47	0.44
2:B:80:LYS:HA	2:B:117:PRO:HG2	1.99	0.43
2:D:85:TRP:CZ3	3:D:1002:LAE:H52	2.53	0.43
2:D:158:ARG:NH1	2:D:162:LEU:CD1	2.81	0.43
2:D:18:GLU:HG2	2:D:22:LYS:HE3	2.00	0.43
2:D:230:ARG:NH2	4:D:1005:HOH:O	2.36	0.43
1:E:10:DA:C2'	1:E:11:DT:H5''	2.48	0.43
1:F:102:DA:H1'	1:F:103:DT:H5'	1.99	0.43
2:A:111:ARG:NH2	2:A:135:PRO:HB3	2.34	0.43
1:G:6:DG:H2''	1:G:7:DC:C5'	2.45	0.43
2:C:91:ARG:O	2:C:93:THR:N	2.51	0.43
1:H:106:DG:H2''	1:H:107:DC:C5'	2.40	0.43
2:A:207:VAL:HA	2:A:210:ARG:HG2	2.00	0.42
2:D:47:ILE:HG13	2:D:62:PHE:HE1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:PHE:CD2	2:D:130:MSE:CG	3.02	0.42
2:C:1:MSE:HE2	2:C:32:PHE:HZ	1.82	0.42
4:F:135:HOH:O	2:C:201:LYS:HE3	2.18	0.42
2:C:4:TRP:HB3	2:C:32:PHE:CD2	2.55	0.42
2:D:7:LYS:NZ	2:D:198:GLU:HA	2.33	0.42
2:A:74:LYS:NZ	2:A:74:LYS:CB	2.82	0.42
2:A:74:LYS:HZ2	2:A:74:LYS:HB2	1.82	0.42
1:F:116:DA:H2''	1:F:117:DC:O5'	2.19	0.42
2:D:158:ARG:HH12	2:D:162:LEU:HD12	1.85	0.42
2:A:40:LEU:O	2:A:126:SER:HA	2.20	0.42
1:E:16:DA:H2''	1:E:17:DC:C5'	2.46	0.42
2:C:95:SER:OG	2:C:98:GLU:HG3	2.20	0.42
2:A:75:ARG:HD3	2:A:83:PHE:CD2	2.55	0.41
2:B:75:ARG:HD3	2:B:83:PHE:CD2	2.55	0.41
2:C:111:ARG:HD2	2:C:133:ASP:O	2.20	0.41
2:B:111:ARG:HD3	2:B:133:ASP:O	2.20	0.41
2:B:90:GLU:O	2:B:94:LEU:HD22	2.20	0.41
2:C:99:ARG:HD3	2:C:99:ARG:C	2.40	0.41
2:D:116:ILE:HB	2:D:152:ILE:HG13	2.01	0.41
2:A:80:LYS:HG2	4:A:1112:HOH:O	2.20	0.41
2:A:17:ASP:OD2	2:A:19:CYS:SG	2.78	0.41
2:D:85:TRP:CH2	3:D:1002:LAE:H52	2.56	0.41
1:F:115:DC:H2''	1:F:116:DA:C5'	2.50	0.41
2:A:12:ALA:HB2	2:A:155:ILE:HD13	2.02	0.41
2:A:182:LEU:HD23	2:A:234:ILE:HD11	2.02	0.41
2:B:39:TYR:OH	2:B:156:HIS:CD2	2.72	0.41
2:C:42:ILE:HG12	2:C:47:ILE:HG22	2.03	0.41
2:C:42:ILE:HG23	2:C:47:ILE:HG22	2.03	0.41
2:C:85:TRP:CH2	3:C:1004:LAE:H52	2.55	0.41
1:H:114:DG:H2''	1:H:115:DC:C5'	2.48	0.41
2:D:91:ARG:HD2	2:D:99:ARG:NE	2.36	0.41
2:A:43:GLN:HG2	2:A:124:PHE:CG	2.56	0.41
2:B:231:ARG:O	2:B:232:LYS:HB2	2.21	0.41
2:D:4:TRP:CE3	2:D:130:MSE:HE2	2.56	0.41
1:H:117:DC:H2''	1:H:118:DA:OP2	2.21	0.41
2:A:42:ILE:HD12	2:A:47:ILE:HD13	2.02	0.41
2:B:182:LEU:CD2	2:B:234:ILE:HD11	2.51	0.41
2:C:90:GLU:O	2:C:94:LEU:HG	2.21	0.41
2:B:191:MSE:HG3	2:B:205:VAL:CG1	2.51	0.40
2:D:101:PHE:CE2	3:D:1002:LAE:H42	2.56	0.40
2:B:17:ASP:OD1	2:B:19:CYS:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:THR:HG23	4:D:1015:HOH:O	2.20	0.40
2:C:190:THR:OG1	2:C:193:GLU:HG3	2.21	0.40
2:D:111:ARG:HD2	2:D:133:ASP:O	2.22	0.40
2:C:91:ARG:HB3	2:C:92:PRO:CD	2.51	0.40
2:A:11:LEU:O	2:A:14:ILE:HG22	2.22	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	
2	A	231/234 (99%)	221 (96%)	9 (4%)	1 (0%)	38	17
2	B	231/234 (99%)	224 (97%)	7 (3%)	0	100	100
2	C	221/234 (94%)	211 (96%)	8 (4%)	2 (1%)	20	4
2	D	221/234 (94%)	214 (97%)	7 (3%)	0	100	100
All	All	904/936 (97%)	870 (96%)	31 (3%)	3 (0%)	44	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	92	PRO
2	A	3	HIS
2	C	95	SER

5.3.2 Protein sidechains [i](#)

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	
2	A	187/189 (99%)	184 (98%)	3 (2%)	68	45
2	B	185/189 (98%)	183 (99%)	2 (1%)	78	61
2	C	188/189 (100%)	183 (97%)	5 (3%)	50	22
2	D	188/189 (100%)	183 (97%)	5 (3%)	50	22
All	All	748/756 (99%)	733 (98%)	15 (2%)	60	36

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	56	GLN
2	A	94	LEU
2	A	139	LEU
2	B	94	LEU
2	B	191	MSE
2	C	47	ILE
2	C	99	ARG
2	C	162	LEU
2	C	198	GLU
2	C	219	ARG
2	D	64	LYS
2	D	99	ARG
2	D	130	MSE
2	D	184	TRP
2	D	211	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	56	GLN
2	A	81	HIS
2	A	104	HIS
2	A	156	HIS
2	B	3	HIS
2	B	56	GLN
2	B	81	HIS
2	B	156	HIS
2	C	3	HIS
2	C	41	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	54	HIS
2	C	156	HIS
2	D	3	HIS
2	D	31	HIS
2	D	41	HIS
2	D	54	HIS
2	D	156	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 ⓘ

4 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	LAE	A	1003	-	17,17,17	1.92	4 (23%)	17,21,21	3.49	7 (41%)
3	LAE	B	1001	-	17,17,17	1.91	4 (23%)	17,21,21	3.48	7 (41%)
3	LAE	C	1004	-	17,17,17	1.97	4 (23%)	17,21,21	3.40	7 (41%)
3	LAE	D	1002	-	17,17,17	2.04	4 (23%)	17,21,21	3.45	7 (41%)

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	LAE	A	1003	-	-	0/13/23/23	0/1/1/1
3	LAE	B	1001	-	-	0/13/23/23	0/1/1/1
3	LAE	C	1004	-	-	0/13/23/23	0/1/1/1
3	LAE	D	1002	-	-	0/13/23/23	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1004	LAE	O3-C2	-2.55	1.29	1.35
3	D	1002	LAE	O3-C2	-2.42	1.29	1.35
3	B	1001	LAE	O3-C2	-2.18	1.30	1.35
3	A	1003	LAE	O3-C2	-2.17	1.30	1.35
3	C	1004	LAE	C13-N11	2.28	1.38	1.34
3	A	1003	LAE	C13-N11	2.40	1.39	1.34
3	B	1001	LAE	C13-N11	2.41	1.39	1.34
3	D	1002	LAE	C13-N11	2.59	1.39	1.34
3	C	1004	LAE	C5-C4	3.12	1.60	1.51
3	B	1001	LAE	C5-C4	3.19	1.60	1.51
3	A	1003	LAE	C5-C4	3.33	1.60	1.51
3	D	1002	LAE	C5-C4	3.48	1.61	1.51
3	B	1001	LAE	O3-C4	5.26	1.59	1.46
3	A	1003	LAE	O3-C4	5.32	1.59	1.46
3	C	1004	LAE	O3-C4	5.63	1.60	1.46
3	D	1002	LAE	O3-C4	5.64	1.60	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	LAE	O3-C4-C5	-6.24	95.29	105.77
3	B	1001	LAE	O3-C4-C5	-6.18	95.40	105.77
3	D	1002	LAE	O3-C4-C5	-6.12	95.50	105.77
3	D	1002	LAE	O35-C13-C14	-6.04	113.07	121.39
3	C	1004	LAE	O3-C4-C5	-5.96	95.77	105.77
3	A	1003	LAE	C1-N11-C13	-5.79	106.33	121.62
3	A	1003	LAE	O35-C13-C14	-5.69	113.57	121.39
3	D	1002	LAE	C1-N11-C13	-5.67	106.64	121.62
3	C	1004	LAE	O35-C13-C14	-5.66	113.60	121.39
3	B	1001	LAE	O35-C13-C14	-5.65	113.61	121.39
3	C	1004	LAE	C1-N11-C13	-5.64	106.72	121.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	LAE	C1-N11-C13	-5.58	106.88	121.62
3	B	1001	LAE	C2-C1-N11	-2.88	107.62	112.36
3	A	1003	LAE	C2-C1-N11	-2.38	108.44	112.36
3	C	1004	LAE	C2-C1-N11	-2.29	108.59	112.36
3	D	1002	LAE	C2-C1-N11	-2.22	108.70	112.36
3	D	1002	LAE	O3-C2-O10	2.75	124.39	121.43
3	C	1004	LAE	O3-C2-O10	2.91	124.56	121.43
3	A	1003	LAE	O3-C2-O10	3.12	124.79	121.43
3	B	1001	LAE	O3-C2-O10	3.28	124.96	121.43
3	A	1003	LAE	O35-C13-N11	3.64	129.26	122.97
3	D	1002	LAE	O35-C13-N11	3.68	129.33	122.97
3	C	1004	LAE	O35-C13-N11	3.71	129.38	122.97
3	B	1001	LAE	O35-C13-N11	4.02	129.92	122.97
3	D	1002	LAE	C4-O3-C2	8.07	118.07	110.42
3	B	1001	LAE	C4-O3-C2	8.07	118.07	110.42
3	C	1004	LAE	C4-O3-C2	8.08	118.08	110.42
3	A	1003	LAE	C4-O3-C2	8.28	118.27	110.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	LAE	2	0
3	B	1001	LAE	1	0
3	C	1004	LAE	2	0
3	D	1002	LAE	3	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.