



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2017 – 01:21 AM EST

PDB ID : 5DG3  
Title : Structure of Pseudomonas aeruginosa LpxA in complex with UDP-3-O-(R-3-hydroxydecanoyl)-GlcNAc  
Authors : Smith, E.W.; Chen, Y.  
Deposited on : unknown  
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
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) : rb-20030345

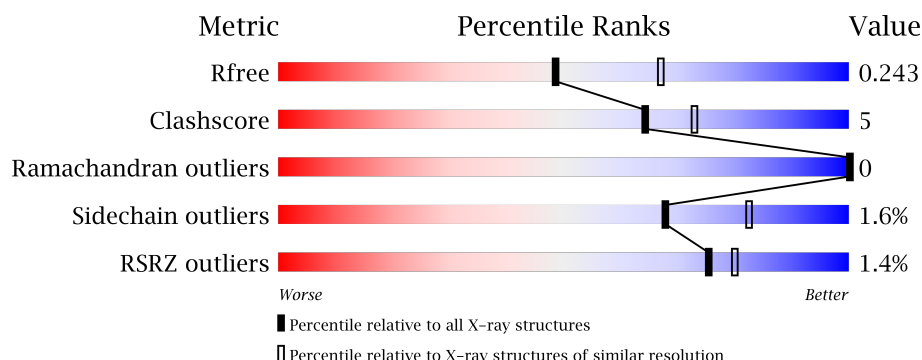
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	258	
1	B	258	
1	C	258	
1	D	258	
1	E	258	

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Mol	Chain	Length	Quality of chain
1	F	258	 88% 11%

2 Entry composition ⓘ

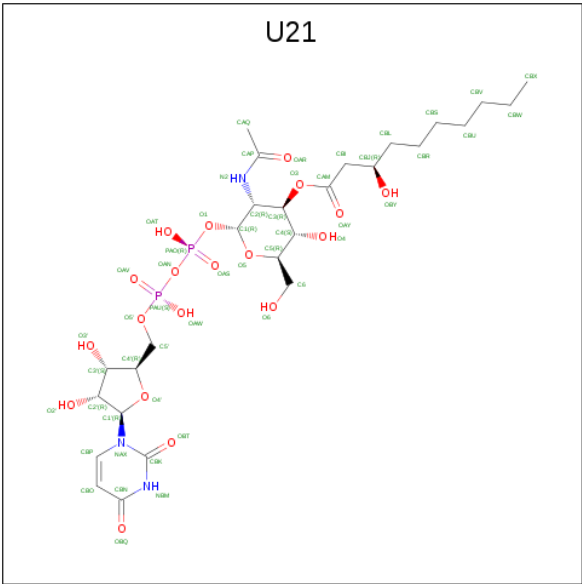
There are 4 unique types of molecules in this entry. The entry contains 12103 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase.

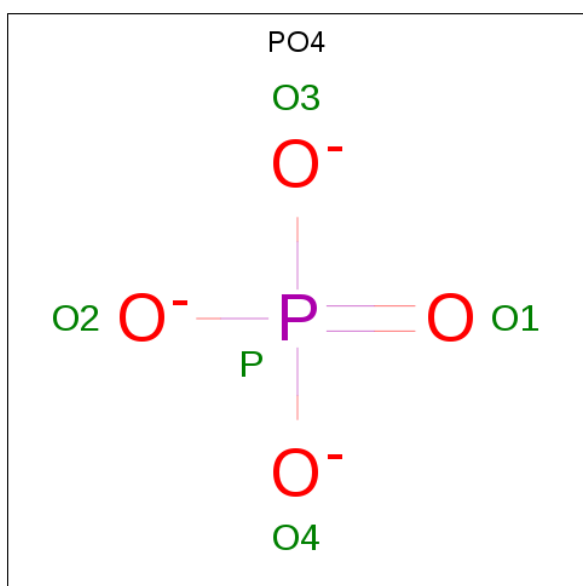
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1944	1217	359	362	6			
1	B	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	C	256	Total	C	N	O	S	0	0	0
			1950	1222	359	363	6			
1	D	249	Total	C	N	O	S	0	0	0
			1889	1183	349	351	6			
1	E	256	Total	C	N	O	S	0	0	0
			1948	1221	359	362	6			
1	F	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			

- Molecule 2 is uridine-5'-diphosphate-3-O-(R-3-hydroxydecanoyl)-N-acetyl-D-glucosamine (three-letter code: U21) (formula: C<sub>27</sub>H<sub>45</sub>N<sub>3</sub>O<sub>19</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			51	27	3	19	2		
2	C	1	Total	C	N	O	P	0	0
			51	27	3	19	2		
2	D	1	Total	C	N	O	P	0	0
			51	27	3	19	2		
2	E	1	Total	C	N	O	P	0	0
			51	27	3	19	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	35	Total	O	0	0
			35	35		
4	C	31	Total	O	0	0
			31	31		
4	D	46	Total	O	0	0
			46	46		
4	E	23	Total	O	0	0
			23	23		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	41	Total	O	0	0
			41	41		

### 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: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain A: 




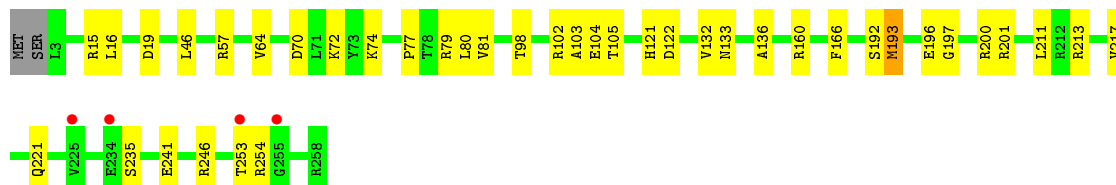
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain B: 




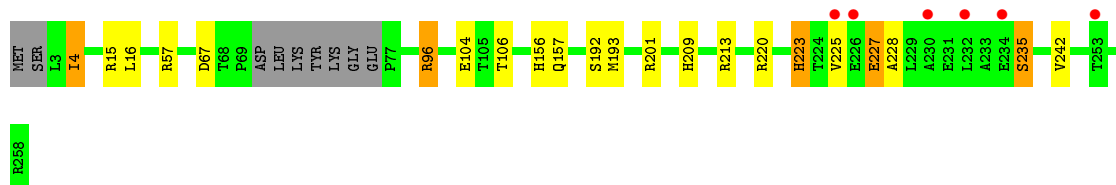
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain C: 

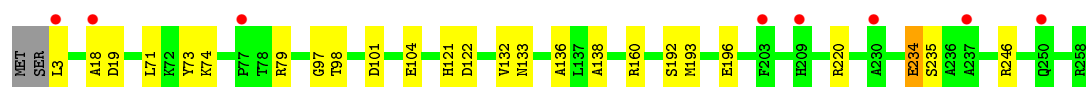
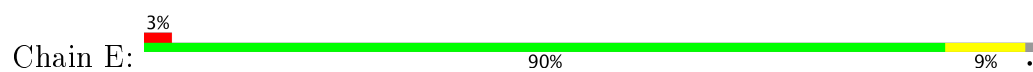


- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

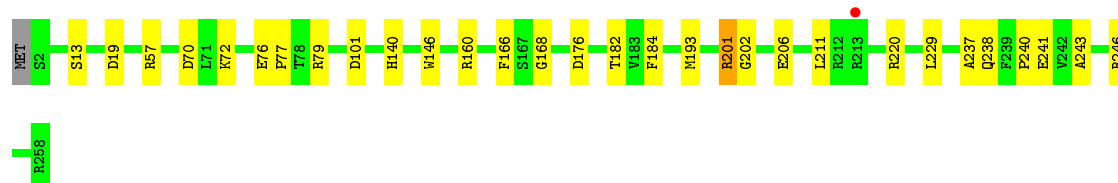
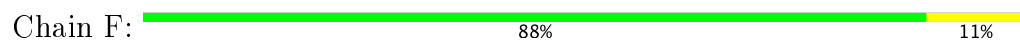
Chain D: 



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.96 Å 83.33 Å 220.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.18 – 2.30 45.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.0 (110.18-2.30) 91.1 (45.96-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.193 , 0.245 0.198 , 0.243	Depositor DCC
$R_{free}$ test set	3035 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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, 0.333 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: PO4, U21

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	0.95	2/1985 (0.1%)	1.02	11/2694 (0.4%)
1	B	0.94	2/2008 (0.1%)	1.04	12/2724 (0.4%)
1	C	0.96	2/1992 (0.1%)	0.96	6/2704 (0.2%)
1	D	1.04	2/1929 (0.1%)	1.03	7/2618 (0.3%)
1	E	0.90	1/1990 (0.1%)	0.89	4/2701 (0.1%)
1	F	0.99	1/2008 (0.0%)	1.13	13/2724 (0.5%)
All	All	0.96	10/11912 (0.1%)	1.01	53/16165 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	96	ARG	CZ-NH1	-10.53	1.19	1.33
1	D	96	ARG	CZ-NH2	-7.99	1.22	1.33
1	B	220	ARG	CZ-NH2	-5.78	1.25	1.33
1	C	166	PHE	CG-CD1	-5.32	1.30	1.38
1	F	160	ARG	CZ-NH1	-5.31	1.26	1.33
1	C	235	SER	CB-OG	-5.26	1.35	1.42
1	E	160	ARG	CZ-NH2	-5.24	1.26	1.33
1	B	160	ARG	CZ-NH1	-5.23	1.26	1.33
1	A	79	ARG	CZ-NH2	-5.17	1.26	1.33
1	A	160	ARG	CZ-NH1	-5.06	1.26	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	201	ARG	NE-CZ-NH2	18.91	129.76	120.30
1	D	96	ARG	NE-CZ-NH2	16.44	128.52	120.30
1	F	220	ARG	NE-CZ-NH1	16.20	128.40	120.30
1	F	201	ARG	NE-CZ-NH1	-13.35	113.63	120.30
1	C	246	ARG	NE-CZ-NH2	13.25	126.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ARG	NE-CZ-NH1	-11.81	114.40	120.30
1	D	57	ARG	NE-CZ-NH1	-11.80	114.40	120.30
1	B	199	ARG	NE-CZ-NH2	-10.67	114.96	120.30
1	F	57	ARG	NE-CZ-NH2	10.44	125.52	120.30
1	B	57	ARG	NE-CZ-NH2	10.43	125.51	120.30
1	D	57	ARG	NE-CZ-NH2	10.24	125.42	120.30
1	B	246	ARG	NE-CZ-NH1	10.17	125.38	120.30
1	A	246	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	D	96	ARG	NH1-CZ-NH2	-9.63	108.81	119.40
1	C	160	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	E	246	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	F	57	ARG	NE-CZ-NH1	-9.08	115.76	120.30
1	A	160	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	F	160	ARG	NE-CZ-NH2	8.87	124.73	120.30
1	F	220	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	E	160	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	175	LYS	CD-CE-NZ	8.03	130.18	111.70
1	C	246	ARG	CD-NE-CZ	7.83	134.56	123.60
1	A	79	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	F	201	ARG	CD-NE-CZ	7.76	134.46	123.60
1	C	246	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	B	160	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	70	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	220	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	160	ARG	NH1-CZ-NH2	-7.17	111.51	119.40
1	A	160	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	B	160	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	11	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	160	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
1	C	160	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	E	160	ARG	NH1-CZ-NH2	-6.21	112.56	119.40
1	A	193	MET	CG-SD-CE	6.10	109.96	100.20
1	F	201	ARG	CG-CD-NE	6.08	124.57	111.80
1	A	200	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	F	70	ASP	CB-CG-OD1	5.96	123.66	118.30
1	D	220	ARG	CG-CD-NE	-5.80	99.62	111.80
1	F	160	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
1	A	201	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	79	ARG	NH1-CZ-NH2	-5.50	113.34	119.40
1	F	176	ASP	CB-CG-OD1	5.43	123.19	118.30
1	F	79	ARG	CB-CA-C	-5.34	99.72	110.40
1	B	36	GLU	OE1-CD-OE2	-5.32	116.92	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	MET	CG-SD-CE	5.29	108.66	100.20
1	E	220	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	201	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	224	THR	N-CA-C	-5.06	97.34	111.00
1	A	76	GLU	C-N-CD	5.01	138.93	128.40
1	D	223	HIS	CB-CA-C	-5.01	100.38	110.40

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	1944	0	1910	29	0
1	B	1966	0	1935	15	0
1	C	1950	0	1915	29	0
1	D	1889	0	1849	13	0
1	E	1948	0	1910	17	0
1	F	1966	0	1935	23	0
2	B	51	0	43	2	0
2	C	51	0	43	6	0
2	D	51	0	43	0	0
2	E	51	0	43	2	0
3	E	5	0	0	0	0
4	A	55	0	0	0	0
4	B	35	0	0	0	0
4	C	31	0	0	0	0
4	D	46	0	0	0	0
4	E	23	0	0	0	0
4	F	41	0	0	0	0
All	All	12103	0	11626	112	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 5.

All (112) 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:235:SER:HB3	1:D:242:VAL:HG11	1.54	0.86
1:A:72:LYS:NZ	1:F:206:GLU:HG2	1.92	0.82
1:C:81:VAL:CG2	1:C:104:GLU:OE2	2.32	0.77
1:A:229:LEU:HD23	1:A:246:ARG:HG2	1.65	0.76
1:C:196:GLU:O	1:C:200:ARG:HG3	1.86	0.75
1:C:200:ARG:HD3	1:F:237:ALA:CB	2.17	0.75
1:F:166:PHE:HB3	1:F:182:THR:HG22	1.72	0.72
1:A:68:THR:OG1	1:A:69:PRO:HD2	1.90	0.71
1:B:250:GLN:O	1:E:18:ALA:HB3	1.91	0.70
1:A:100:GLN:NE2	1:F:241:GLU:HG3	2.08	0.69
1:C:72:LYS:NZ	2:C:301:U21:O6	2.23	0.68
1:B:174:GLY:O	1:B:254:ARG:NH2	2.26	0.68
1:D:225:VAL:O	1:D:228:ALA:HB3	1.94	0.67
1:C:81:VAL:HG23	1:C:104:GLU:OE2	1.93	0.67
1:B:166:PHE:HB3	1:B:182:THR:HG22	1.76	0.67
1:B:19:ASP:N	1:B:19:ASP:OD1	2.21	0.66
1:C:200:ARG:HD3	1:F:237:ALA:HB2	1.80	0.64
1:A:72:LYS:HZ1	1:F:206:GLU:HG2	1.63	0.63
1:C:72:LYS:O	1:C:74:LYS:HD2	1.99	0.63
1:D:15:ARG:O	1:D:16:LEU:HD12	1.98	0.63
1:C:136:ALA:CB	2:C:301:U21:HBW2	2.29	0.62
1:C:253:THR:HG23	1:C:254:ARG:N	2.14	0.62
1:A:225:VAL:O	1:A:229:LEU:HD12	2.00	0.61
1:C:200:ARG:HD3	1:F:237:ALA:HB1	1.82	0.61
1:C:197:GLY:O	1:C:201:ARG:HD2	2.00	0.61
1:D:67:ASP:OD1	1:D:96:ARG:NH2	2.31	0.61
1:C:136:ALA:HB1	2:C:301:U21:HBW2	1.82	0.60
1:A:76:GLU:N	1:A:76:GLU:OE1	2.27	0.59
1:C:81:VAL:HG21	1:C:104:GLU:OE2	2.03	0.58
1:C:79:ARG:NH1	1:C:104:GLU:OE1	2.35	0.57
1:E:192:SER:OG	1:E:193:MET:N	2.37	0.56
1:D:67:ASP:OD1	1:D:96:ARG:NH1	2.38	0.56
1:A:225:VAL:HG13	1:A:229:LEU:CD1	2.36	0.56
1:A:166:PHE:HB3	1:A:182:THR:HG22	1.87	0.56
1:D:4:ILE:HD11	1:D:16:LEU:HD23	1.88	0.55
1:D:209:HIS:O	1:D:213:ARG:HG3	2.06	0.55
1:A:225:VAL:HG13	1:A:229:LEU:HD12	1.89	0.54
1:A:229:LEU:HD23	1:A:246:ARG:CG	2.35	0.54
1:A:72:LYS:HZ2	1:F:206:GLU:HG2	1.73	0.54
1:A:100:GLN:HE21	1:F:241:GLU:HG3	1.72	0.53
1:C:253:THR:HG23	1:C:254:ARG:H	1.71	0.53
1:A:74:LYS:HB2	1:A:76:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:SER:OG	1:D:193:MET:N	2.41	0.52
1:B:133:ASN:HB2	2:C:301:U21:HBU1	1.92	0.52
1:A:77:PRO:HD2	1:F:202:GLY:HA3	1.91	0.51
1:E:98:THR:OG1	1:E:122:ASP:OD2	2.25	0.51
1:F:146:TRP:CE3	1:F:201:ARG:HD3	2.45	0.50
1:D:4:ILE:CD1	1:D:16:LEU:HD23	2.41	0.50
1:C:192:SER:OG	1:C:193:MET:N	2.43	0.50
1:E:19:ASP:OD1	1:E:19:ASP:N	2.37	0.50
1:D:104:GLU:OE2	1:D:106:THR:OG1	2.26	0.50
1:B:102:ARG:NH2	1:B:104:GLU:O	2.45	0.50
1:B:61:PHE:O	1:B:91:GLY:HA2	2.11	0.50
1:A:61:PHE:O	1:A:91:GLY:HA2	2.13	0.49
1:B:180:TYR:HB3	1:B:198:MET:HE2	1.94	0.49
1:F:19:ASP:OD1	1:F:19:ASP:N	2.40	0.49
1:F:101:ASP:OD2	1:F:140:HIS:ND1	2.41	0.49
1:C:70:ASP:OD1	1:C:72:LYS:HE3	2.12	0.49
1:A:221:GLN:HB2	1:A:223:HIS:HD2	1.78	0.48
1:C:98:THR:O	1:C:103:ALA:N	2.47	0.48
1:E:79:ARG:NH1	1:E:104:GLU:OE1	2.43	0.48
1:F:168:GLY:HA3	1:F:184:PHE:CE2	2.49	0.48
1:A:100:GLN:CD	1:A:100:GLN:H	2.17	0.48
1:E:136:ALA:HB1	2:E:301:U21:HBV2	1.96	0.48
1:D:15:ARG:C	1:D:16:LEU:HD12	2.35	0.48
1:E:234:GLU:HG2	1:E:235:SER:N	2.28	0.47
1:B:138:ALA:O	2:B:301:U21:HBJ	2.13	0.47
1:A:151:GLY:HA3	2:B:301:U21:HBV1	1.97	0.47
1:E:97:GLY:HA2	1:E:122:ASP:OD1	2.14	0.47
1:A:72:LYS:NZ	1:F:206:GLU:CG	2.73	0.46
1:B:226:GLU:OE2	1:E:3:LEU:HG	2.16	0.45
1:D:223:HIS:HB3	1:D:227:GLU:HB3	1.99	0.45
1:A:68:THR:OG1	1:A:69:PRO:CD	2.64	0.44
1:A:76:GLU:CG	1:F:202:GLY:O	2.65	0.44
1:E:73:TYR:C	1:E:74:LYS:HG2	2.37	0.44
1:C:217:VAL:HA	1:C:221:GLN:NE2	2.32	0.44
1:A:221:GLN:HB2	1:A:223:HIS:CD2	2.52	0.44
1:C:211:LEU:HD11	1:C:241:GLU:HB3	2.00	0.44
1:F:168:GLY:HA3	1:F:184:PHE:CD2	2.53	0.44
1:A:110:HIS:O	1:A:128:HIS:HA	2.19	0.43
1:C:19:ASP:N	1:C:19:ASP:OD1	2.37	0.43
1:A:46:LEU:HD23	1:A:64:VAL:HB	2.00	0.43
1:B:72:LYS:HE2	1:B:72:LYS:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:PRO:O	1:F:243:ALA:N	2.52	0.43
1:B:151:GLY:HA3	2:C:301:U21:HBV2	2.01	0.42
1:A:192:SER:OG	1:A:193:MET:N	2.52	0.42
1:C:98:THR:O	1:C:103:ALA:HA	2.19	0.42
1:E:71:LEU:HA	1:E:71:LEU:HD23	1.80	0.42
1:E:101:ASP:HB3	1:E:122:ASP:OD2	2.19	0.42
1:C:15:ARG:C	1:C:16:LEU:HD12	2.39	0.42
1:E:234:GLU:CG	1:E:235:SER:N	2.82	0.42
1:C:132:VAL:HG12	1:C:133:ASN:N	2.35	0.41
1:D:156:HIS:CD2	1:D:157:GLN:OE1	2.73	0.41
1:A:219:TYR:HE1	1:A:258:ARG:HA	1.84	0.41
1:E:121:HIS:O	1:E:122:ASP:HB2	2.20	0.41
1:A:76:GLU:HG3	1:F:202:GLY:O	2.21	0.41
1:B:166:PHE:O	1:B:182:THR:HA	2.21	0.41
1:C:46:LEU:HD23	1:C:64:VAL:HB	2.02	0.41
1:A:221:GLN:CB	1:A:223:HIS:CD2	3.04	0.41
1:C:136:ALA:HB3	2:C:301:U21:HBW2	2.01	0.41
1:F:76:GLU:HB3	1:F:77:PRO:HD2	2.01	0.41
1:E:138:ALA:HA	2:E:301:U21:HBS1	2.02	0.41
1:C:121:HIS:O	1:C:122:ASP:HB2	2.21	0.41
1:C:253:THR:CG2	1:C:254:ARG:N	2.82	0.40
1:E:132:VAL:HG12	1:E:133:ASN:N	2.36	0.40
1:F:72:LYS:HE2	1:F:72:LYS:HB2	1.71	0.40
1:B:72:LYS:O	1:B:74:LYS:HG2	2.22	0.40
1:C:80:LEU:HA	1:C:105:THR:O	2.22	0.40
1:F:211:LEU:HD23	1:F:211:LEU:HA	1.85	0.40
1:F:229:LEU:HD23	1:F:246:ARG:HG2	2.02	0.40
1:E:97:GLY:CA	1:E:122:ASP:OD1	2.70	0.40
1:B:213:ARG:HH11	1:B:221:GLN:HE22	1.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/258 (98%)	239 (94%)	15 (6%)	0	100	100
1	B	255/258 (99%)	244 (96%)	11 (4%)	0	100	100
1	C	254/258 (98%)	236 (93%)	18 (7%)	0	100	100
1	D	245/258 (95%)	232 (95%)	13 (5%)	0	100	100
1	E	254/258 (98%)	245 (96%)	9 (4%)	0	100	100
1	F	255/258 (99%)	241 (94%)	14 (6%)	0	100	100
All	All	1517/1548 (98%)	1437 (95%)	80 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	201/206 (98%)	198 (98%)	3 (2%)	70	83
1	B	205/206 (100%)	201 (98%)	4 (2%)	60	77
1	C	202/206 (98%)	198 (98%)	4 (2%)	60	77
1	D	195/206 (95%)	192 (98%)	3 (2%)	70	83
1	E	201/206 (98%)	199 (99%)	2 (1%)	80	90
1	F	205/206 (100%)	202 (98%)	3 (2%)	70	83
All	All	1209/1236 (98%)	1190 (98%)	19 (2%)	68	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	220	ARG
1	A	225	VAL
1	B	123	SER
1	B	201	ARG
1	B	205	SER
1	B	226	GLU

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Mol	Chain	Res	Type
1	C	57	ARG
1	C	77	PRO
1	C	102	ARG
1	C	213	ARG
1	D	4	ILE
1	D	227	GLU
1	D	235	SER
1	E	196	GLU
1	E	234	GLU
1	F	13	SER
1	F	193	MET
1	F	238	GLN

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	223	HIS
1	A	238	GLN
1	B	221	GLN
1	C	221	GLN
1	C	238	GLN
1	D	221	GLN
1	D	238	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 ⓘ

5 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	U21	B	301	-	46,53,53	1.85	14 (30%)	56,76,76	1.75	8 (14%)
2	U21	C	301	-	46,53,53	1.57	11 (23%)	56,76,76	1.72	7 (12%)
2	U21	D	301	-	46,53,53	0.88	2 (4%)	56,76,76	1.42	2 (3%)
2	U21	E	301	-	46,53,53	1.79	15 (32%)	56,76,76	1.67	10 (17%)
3	PO4	E	302	-	4,4,4	1.69	0	6,6,6	1.22	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
2	U21	B	301	-	-	0/37/78/78	0/3/3/3
2	U21	C	301	-	-	0/37/78/78	0/3/3/3
2	U21	D	301	-	-	0/37/78/78	0/3/3/3
2	U21	E	301	-	-	0/37/78/78	0/3/3/3
3	PO4	E	302	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	U21	CBK-NBM	-4.62	1.29	1.38
2	E	301	U21	CBP-NAX	-4.35	1.29	1.35
2	E	301	U21	CBK-NBM	-3.77	1.30	1.38
2	B	301	U21	PAO-O1	-3.76	1.51	1.60
2	E	301	U21	O3-C3	-3.69	1.39	1.44
2	B	301	U21	CBP-NAX	-3.56	1.31	1.35
2	C	301	U21	O3-C3	-3.50	1.39	1.44
2	B	301	U21	O3-C3	-3.41	1.39	1.44
2	C	301	U21	CBK-NBM	-3.33	1.31	1.38
2	B	301	U21	PAO-OAS	-3.32	1.38	1.50
2	B	301	U21	PAU-OAW	-3.30	1.38	1.55
2	B	301	U21	PAO-OAT	-3.06	1.39	1.55
2	E	301	U21	PAO-O1	-2.97	1.53	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	U21	PAO-OAT	-2.91	1.40	1.55
2	C	301	U21	C2'-C1'	-2.75	1.49	1.53
2	E	301	U21	PAO-OAS	-2.66	1.40	1.50
2	B	301	U21	OAR-CAP	-2.65	1.17	1.23
2	D	301	U21	CBK-NBM	-2.64	1.32	1.38
2	C	301	U21	CBP-NAX	-2.55	1.32	1.35
2	E	301	U21	PAU-OAV	-2.50	1.41	1.50
2	E	301	U21	C2-N2	-2.48	1.41	1.45
2	C	301	U21	C2-N2	-2.45	1.41	1.45
2	C	301	U21	O5-C5	-2.29	1.38	1.44
2	B	301	U21	C2'-C1'	-2.28	1.50	1.53
2	E	301	U21	CAQ-CAP	-2.27	1.45	1.50
2	E	301	U21	O5-C5	-2.22	1.39	1.44
2	C	301	U21	O4'-C4'	-2.16	1.40	1.45
2	E	301	U21	OAR-CAP	-2.14	1.18	1.23
2	B	301	U21	C1-C2	-2.13	1.49	1.53
2	E	301	U21	PAU-OAW	-2.10	1.44	1.55
2	C	301	U21	O4'-C1'	-2.08	1.38	1.41
2	C	301	U21	C1-C2	-2.08	1.49	1.53
2	B	301	U21	C2-N2	-2.07	1.42	1.45
2	E	301	U21	CBN-NBM	-2.06	1.29	1.33
2	B	301	U21	O5-C5	-2.05	1.39	1.44
2	C	301	U21	PAO-OAT	-2.05	1.44	1.55
2	E	301	U21	OBY-CBJ	-2.02	1.37	1.43
2	B	301	U21	PAU-OAV	-2.01	1.43	1.50
2	E	301	U21	O3-CAM	3.05	1.43	1.34
2	B	301	U21	O3-CAM	3.27	1.43	1.34
2	D	301	U21	O3-CAM	3.63	1.44	1.34
2	C	301	U21	O3-CAM	3.64	1.44	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	U21	C1-C2-N2	-5.69	101.41	111.03
2	B	301	U21	C1-C2-N2	-4.91	102.72	111.03
2	B	301	U21	OAN-PAO-O1	-4.12	94.68	102.05
2	D	301	U21	OAN-PAO-O1	-3.97	94.95	102.05
2	E	301	U21	O5-C1-O1	-3.50	106.78	111.36
2	C	301	U21	OAN-PAO-O1	-3.26	96.22	102.05
2	C	301	U21	O1-C1-C2	-2.96	103.05	108.40
2	B	301	U21	O2'-C2'-C3'	-2.37	104.23	111.83
2	E	301	U21	OAY-CAM-CBI	-2.30	119.51	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	U21	OAR-CAP-CAQ	-2.17	118.10	122.06
2	E	301	U21	O2'-C2'-C3'	-2.13	105.01	111.83
2	E	301	U21	O4'-C1'-NAX	-2.06	103.95	108.08
2	E	301	U21	OAR-CAP-CAQ	-2.04	118.34	122.06
2	B	301	U21	C3-C2-N2	2.14	114.76	111.00
2	E	301	U21	OAW-PAU-OAV	2.15	123.42	112.28
2	C	301	U21	C1-O5-C5	2.30	118.04	113.72
2	C	301	U21	C4'-O4'-C1'	2.39	112.31	109.77
2	E	301	U21	C1-O5-C5	2.48	118.39	113.72
2	B	301	U21	C1-O5-C5	2.52	118.47	113.72
2	E	301	U21	O3-C3-C2	2.72	113.24	107.98
2	C	301	U21	O3-CAM-CBI	3.19	117.45	111.47
2	B	301	U21	O3-CAM-CBI	3.44	117.92	111.47
2	E	301	U21	O3-CAM-CBI	4.45	119.81	111.47
2	C	301	U21	CBN-NBM-CBK	6.70	119.89	114.13
2	D	301	U21	CBN-NBM-CBK	7.05	120.19	114.13
2	E	301	U21	CBN-NBM-CBK	7.08	120.21	114.13
2	B	301	U21	CBN-NBM-CBK	7.60	120.66	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	U21	2	0
2	C	301	U21	6	0
2	E	301	U21	2	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	256/258 (99%)	-0.25	1 (0%) 92 95	13, 26, 49, 50	0
1	B	257/258 (99%)	-0.10	2 (0%) 86 89	18, 33, 48, 50	0
1	C	256/258 (99%)	-0.17	4 (1%) 72 77	15, 32, 50, 50	0
1	D	249/258 (96%)	-0.18	6 (2%) 59 66	12, 30, 49, 50	0
1	E	256/258 (99%)	-0.01	8 (3%) 49 56	14, 35, 50, 50	0
1	F	257/258 (99%)	-0.20	1 (0%) 92 95	11, 28, 50, 50	0
All	All	1531/1548 (98%)	-0.15	22 (1%) 75 80	11, 31, 50, 50	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	237	ALA	5.3
1	D	232	LEU	3.6
1	E	230	ALA	3.5
1	C	253	THR	3.3
1	B	18	ALA	3.2
1	D	253	THR	2.8
1	D	234	GLU	2.7
1	C	255	GLY	2.7
1	B	224	THR	2.6
1	C	234	GLU	2.6
1	D	226	GLU	2.5
1	D	225	VAL	2.3
1	E	3	LEU	2.3
1	E	77	PRO	2.2
1	D	230	ALA	2.2
1	F	213	ARG	2.2
1	A	221	GLN	2.1
1	E	250	GLN	2.1
1	C	225	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	209	HIS	2.0
1	E	203	PHE	2.0
1	E	18	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, 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	PO4	E	302	5/5	0.91	0.16	1.16	47,49,50,50	0
2	U21	C	301	51/51	0.94	0.11	-0.36	27,36,42,45	0
2	U21	E	301	51/51	0.96	0.10	-0.43	22,27,35,37	0
2	U21	D	301	51/51	0.97	0.10	-0.91	15,23,29,29	0
2	U21	B	301	51/51	0.97	0.09	-1.08	20,27,35,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.