



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:52 PM GMT

PDB ID : 4GCV
Title : Structure of a Putative transcription factor (PA1374) from *Pseudomonas aeruginosa*
Authors : Choe, J.; Kim, H.
Deposited on : 2012-07-31
Resolution : 2.30 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 (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

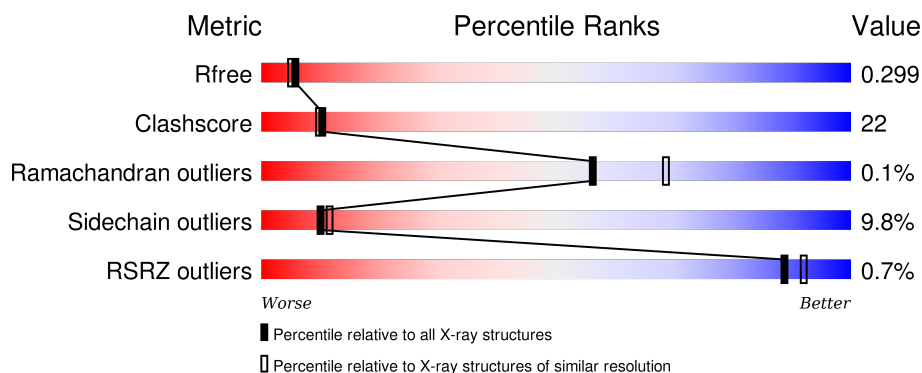
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 ≥ 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	168	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>31%</div> <div>5%</div> <div>14%</div> </div> </div>
1	B	168	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>27%</div> <div>5%</div> <div>13%</div> </div> </div>
1	C	168	<div> <div></div> <div> <div></div> <div>60%</div> <div>21%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	168	<div> <div></div> <div> <div></div> <div>55%</div> <div>26%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	168	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>27%</div> <div>•</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	168	
1	G	168	
1	H	168	
1	I	168	
1	J	168	
1	K	168	
1	L	168	

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
2	NA	A	201	-	-	-	X
2	NA	B	201	-	-	-	X
2	NA	E	201	-	-	-	X
2	NA	F	201	-	-	-	X
2	NA	G	201	-	-	-	X
2	NA	H	201	-	-	-	X
2	NA	J	201	-	-	-	X
2	NA	K	201	-	-	-	X
2	NA	L	201	-	-	-	X
3	GOL	B	205	-	-	X	X
3	GOL	D	203	-	-	-	X
3	GOL	I	202	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14604 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 Putative transcription protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	Se	0	0	0
			1163	727	222	207	2	5			
1	B	146	Total	C	N	O	S	Se	0	0	0
			1171	733	223	208	2	5			
1	C	141	Total	C	N	O	S	Se	0	0	0
			1125	705	211	202	2	5			
1	D	141	Total	C	N	O	S	Se	0	0	0
			1125	705	211	202	2	5			
1	E	142	Total	C	N	O	S	Se	0	0	0
			1134	710	213	204	2	5			
1	F	146	Total	C	N	O	S	Se	0	0	0
			1171	733	223	208	2	5			
1	G	141	Total	C	N	O	S	Se	0	0	0
			1125	705	211	202	2	5			
1	H	146	Total	C	N	O	S	Se	0	0	0
			1171	733	223	208	2	5			
1	I	141	Total	C	N	O	S	Se	0	0	0
			1125	705	211	202	2	5			
1	J	141	Total	C	N	O	S	Se	0	0	0
			1125	705	211	202	2	5			
1	K	146	Total	C	N	O	S	Se	0	0	0
			1171	733	223	208	2	5			
1	L	141	Total	C	N	O	S	Se	0	0	0
			1125	705	211	202	2	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
A	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
B	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
B	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
C	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
D	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
D	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
E	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
E	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
F	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
F	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
G	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
G	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
H	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
H	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
I	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
I	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
J	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
J	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
K	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
K	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
L	106	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0
L	107	GLN	GLU	ENGINEERED MUTATION	UNP Q9I3X0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	K	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	L	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total	Na	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



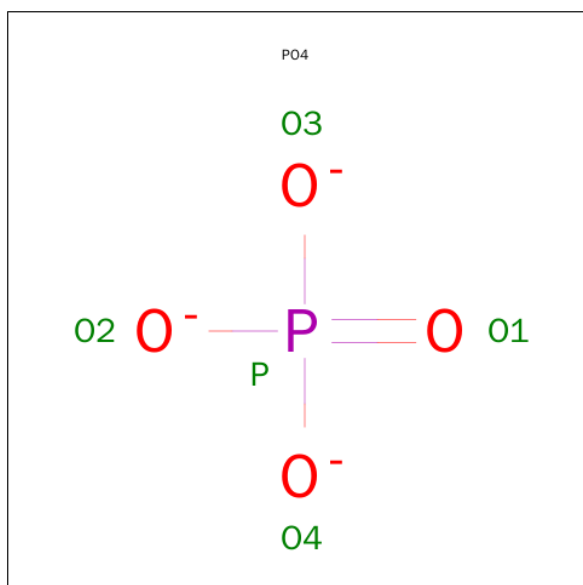
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

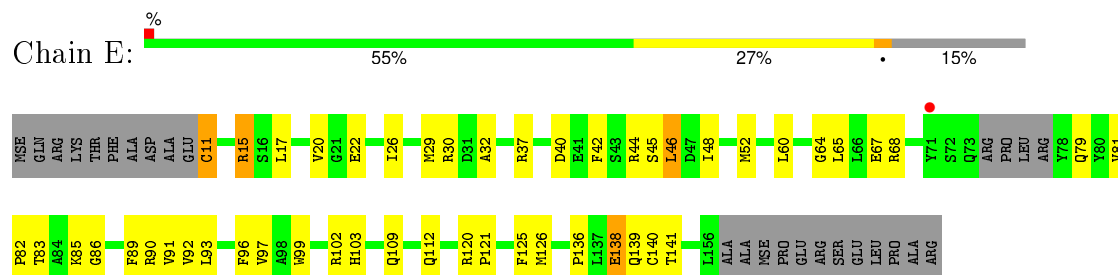
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		
5	B	79	Total	O	0	0
			79	79		
5	C	76	Total	O	0	0
			76	76		

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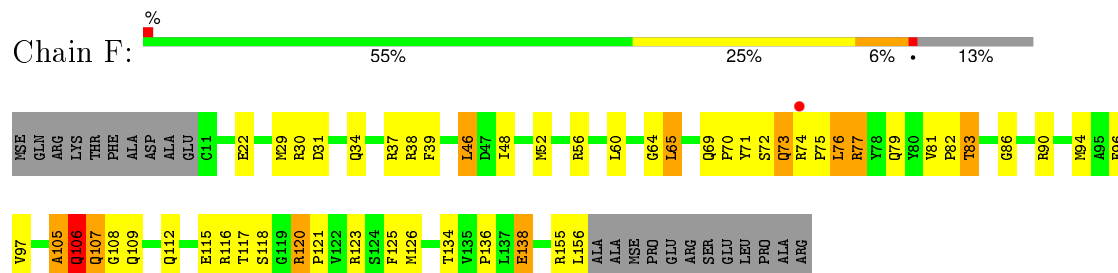
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	73	Total 73	O 73	0	0
5	E	72	Total 72	O 72	0	0
5	F	85	Total 85	O 85	0	0
5	G	68	Total 68	O 68	0	0
5	H	71	Total 71	O 71	0	0
5	I	70	Total 70	O 70	0	0
5	J	60	Total 60	O 60	0	0
5	K	23	Total 23	O 23	0	0
5	L	22	Total 22	O 22	0	0

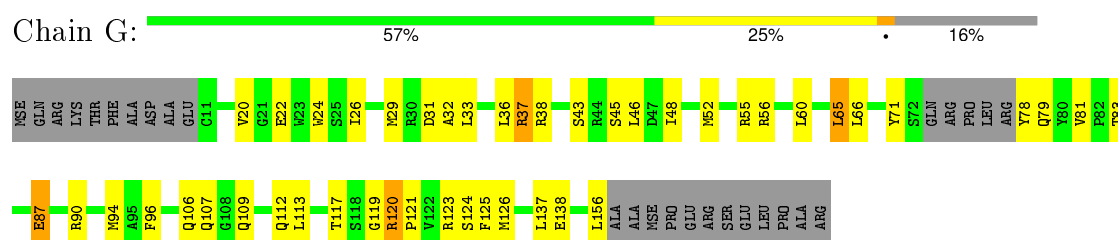
- Molecule 1: Putative transcription protein



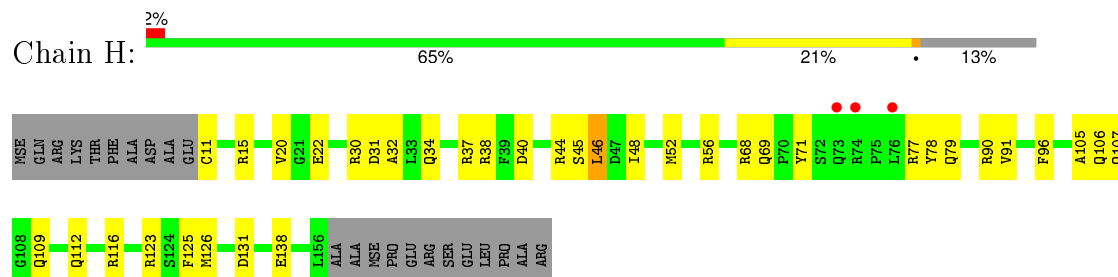
- Molecule 1: Putative transcription protein



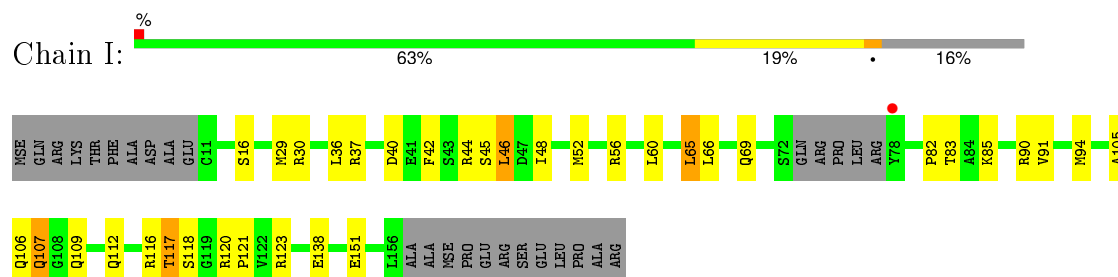
- Molecule 1: Putative transcription protein



- Molecule 1: Putative transcription protein



- Molecule 1: Putative transcription protein



[illegible]

Chain K:

Sequence logo for Chain K showing amino acid conservation across 1412 positions. The y-axis represents information content in bits. The x-axis shows positions 1 to 1412. A color scale at the top indicates conservation levels: 2% (red), 62% (green), 21% (yellow), and 13% (grey). The sequence is displayed in two rows. The first row contains: MSE, GLN, ARG, LYS, THR, PHE, ALA, ASP, ALA, GLU, G11, V20, G21, E22, M29, A32, R37, R44, S45, L46, R56, L60, G64, L65, R68, Y71, S72, Q73, R74, P75, L76, R77, Y78, Q79, Y80, P82, T83, G86, M94, A95, F96, V97, Q109, Q112, L142. The second row contains: V114, E115, S118, G119, A120, R123, S124, F125, M126, T134, V135, P136, L137, E138, R153, L156, ALA, ALA, MSE, PRO, PRO, GLU, ARG, SER, GLU, LEU, PRO, PRO, ALA, ARG.

Chain L:

60% 23% 16%

MSE GLN ARG LYS THR PHE ALA ASP ALA GLU C11 V20 G21 E22 I26 M29 R30 D31 A32 R37 R44 S45 L46 D47 L48 M52 R56 L60 G64 L65 Q69 S72 GLN ARG PRO LEU ARG Y78 Q79 Y80 V81 P82 T83 G86 L93 F96

R102 H103 Q106 Q109 Q112 E115 R116 T117 S118 G119 R120 P121 H122 R123 S124 F125 M126 E138 Q139 C140 E151 L156 ALA ALA MSE PRO PRO GLU ARG SER GLU LEU PRO PRO ALA ALA ARG

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.90Å 74.45Å 230.49Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	29.72 – 2.30 29.72 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.72-2.30) 99.0 (29.72-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.287 0.227 , 0.299	Depositor DCC
R_{free} test set	4863 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.7	EDS
Estimated twinning fraction	0.045 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.044 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.488 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.488 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.039 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 96275 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14604	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.60 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9908e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: GOL, PO4, NA

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	0.79	0/1180	0.85	1/1585 (0.1%)
1	B	0.83	0/1189	0.91	2/1599 (0.1%)
1	C	0.77	0/1141	0.86	4/1533 (0.3%)
1	D	0.78	0/1141	0.87	1/1533 (0.1%)
1	E	0.79	0/1150	0.88	0/1545
1	F	0.86	1/1189 (0.1%)	0.95	3/1599 (0.2%)
1	G	0.74	0/1141	0.86	2/1533 (0.1%)
1	H	0.75	0/1189	0.85	2/1599 (0.1%)
1	I	0.74	0/1141	0.87	1/1533 (0.1%)
1	J	0.75	0/1141	0.86	1/1533 (0.1%)
1	K	0.84	0/1189	0.90	2/1599 (0.1%)
1	L	0.83	1/1141 (0.1%)	0.89	0/1533
All	All	0.79	2/13932 (0.0%)	0.88	19/18724 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	G	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	138	GLU	CG-CD	5.27	1.59	1.51
1	F	107	GLN	CG-CD	5.01	1.62	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	H	56	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	G	37	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	I	56	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	D	133	ARG	NE-CZ-NH2	-6.36	117.12	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	119	GLY	Peptide
1	G	119	GLY	Peptide

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	1163	0	1163	60	0
1	B	1171	0	1175	61	0
1	C	1125	0	1122	47	0
1	D	1125	0	1122	54	0
1	E	1134	0	1130	59	0
1	F	1171	0	1175	69	0
1	G	1125	0	1122	55	0
1	H	1171	0	1175	29	0
1	I	1125	0	1122	45	0
1	J	1125	0	1122	62	0
1	K	1171	0	1175	42	0
1	L	1125	0	1122	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	6	0	8	0	0
3	B	18	0	24	7	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
3	I	6	0	8	0	0
3	J	6	0	8	2	0
3	K	6	0	8	1	0
3	L	6	0	8	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	F	5	0	0	0	0
4	K	5	0	0	0	0
5	A	71	0	0	21	0
5	B	79	0	0	20	0
5	C	76	0	0	9	0
5	D	73	0	0	8	0
5	E	72	0	0	14	0
5	F	85	0	0	24	0
5	G	68	0	0	13	0
5	H	71	0	0	5	0
5	I	70	0	0	9	0
5	J	60	0	0	16	0
5	K	23	0	0	3	0
5	L	22	0	0	2	0
All	All	14604	0	13821	598	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 22.

The worst 5 of 598 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:E:65:LEU:HG	5:E:361:HOH:O	1.32	1.28
1:E:91:VAL:HB	5:F:336:HOH:O	1.22	1.25
1:A:91:VAL:HB	5:A:321:HOH:O	1.09	1.24
1:B:123:ARG:NH1	5:B:358:HOH:O	1.72	1.20
1:F:52:MSE:HG2	5:F:311:HOH:O	1.43	1.18

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	141/168 (84%)	136 (96%)	5 (4%)	0	100	100
1	B	144/168 (86%)	141 (98%)	3 (2%)	0	100	100
1	C	137/168 (82%)	134 (98%)	3 (2%)	0	100	100
1	D	137/168 (82%)	136 (99%)	1 (1%)	0	100	100
1	E	138/168 (82%)	133 (96%)	5 (4%)	0	100	100
1	F	144/168 (86%)	137 (95%)	6 (4%)	1 (1%)	26	31
1	G	137/168 (82%)	134 (98%)	3 (2%)	0	100	100
1	H	144/168 (86%)	142 (99%)	2 (1%)	0	100	100
1	I	137/168 (82%)	131 (96%)	6 (4%)	0	100	100
1	J	137/168 (82%)	133 (97%)	4 (3%)	0	100	100
1	K	144/168 (86%)	138 (96%)	6 (4%)	0	100	100
1	L	137/168 (82%)	133 (97%)	4 (3%)	0	100	100
All	All	1677/2016 (83%)	1628 (97%)	48 (3%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	106	GLN

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	
1	A	121/132 (92%)	104 (86%)	17 (14%)	4	4
1	B	122/132 (92%)	106 (87%)	16 (13%)	5	5
1	C	117/132 (89%)	105 (90%)	12 (10%)	9	10
1	D	117/132 (89%)	107 (92%)	10 (8%)	13	16
1	E	118/132 (89%)	110 (93%)	8 (7%)	20	25
1	F	122/132 (92%)	111 (91%)	11 (9%)	12	14
1	G	117/132 (89%)	106 (91%)	11 (9%)	11	12
1	H	122/132 (92%)	118 (97%)	4 (3%)	45	61
1	I	117/132 (89%)	107 (92%)	10 (8%)	13	16
1	J	117/132 (89%)	102 (87%)	15 (13%)	5	5
1	K	122/132 (92%)	106 (87%)	16 (13%)	5	5
1	L	117/132 (89%)	107 (92%)	10 (8%)	13	16
All	All	1429/1584 (90%)	1289 (90%)	140 (10%)	10	11

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	46	LEU
1	G	65	LEU
1	K	120	ARG
1	F	73	GLN
1	F	106	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	109	GLN
1	G	109	GLN
1	L	69	GLN
1	G	79	GLN
1	H	106	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 11 are monoatomic - leaving 16 for Mogul analysis.

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	GOL	A	202	-	5,5,5	0.31	0	5,5,5	0.66	0
4	PO4	B	202	-	4,4,4	0.22	0	6,6,6	0.29	0
3	GOL	B	203	-	5,5,5	0.43	0	5,5,5	0.51	0
3	GOL	B	204	-	5,5,5	0.36	0	5,5,5	0.50	0
3	GOL	B	205	-	5,5,5	0.48	0	5,5,5	0.46	0
3	GOL	C	201	-	5,5,5	0.20	0	5,5,5	0.65	0
4	PO4	D	202	-	4,4,4	0.43	0	6,6,6	0.29	0
3	GOL	D	203	-	5,5,5	0.37	0	5,5,5	0.48	0
4	PO4	F	202	-	4,4,4	0.29	0	6,6,6	0.28	0
3	GOL	G	202	-	5,5,5	0.47	0	5,5,5	0.37	0
3	GOL	H	202	-	5,5,5	0.21	0	5,5,5	0.60	0
3	GOL	I	202	-	5,5,5	0.22	0	5,5,5	0.74	0
3	GOL	J	202	-	5,5,5	0.32	0	5,5,5	0.73	0
4	PO4	K	202	-	4,4,4	0.33	0	6,6,6	0.28	0
3	GOL	K	203	-	5,5,5	0.51	0	5,5,5	0.45	0
3	GOL	L	202	-	5,5,5	0.19	0	5,5,5	0.58	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	GOL	A	202	-	-	0/4/4/4	0/0/0/0
4	PO4	B	202	-	-	0/0/0/0	0/0/0/0
3	GOL	B	203	-	-	0/4/4/4	0/0/0/0
3	GOL	B	204	-	-	0/4/4/4	0/0/0/0
3	GOL	B	205	-	-	0/4/4/4	0/0/0/0
3	GOL	C	201	-	-	0/4/4/4	0/0/0/0
4	PO4	D	202	-	-	0/0/0/0	0/0/0/0
3	GOL	D	203	-	-	0/4/4/4	0/0/0/0
4	PO4	F	202	-	-	0/0/0/0	0/0/0/0
3	GOL	G	202	-	-	0/4/4/4	0/0/0/0
3	GOL	H	202	-	-	0/4/4/4	0/0/0/0
3	GOL	I	202	-	-	0/4/4/4	0/0/0/0
3	GOL	J	202	-	-	0/4/4/4	0/0/0/0
4	PO4	K	202	-	-	0/0/0/0	0/0/0/0
3	GOL	K	203	-	-	0/4/4/4	0/0/0/0
3	GOL	L	202	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	GOL	1	0
3	B	204	GOL	2	0
3	B	205	GOL	4	0
3	J	202	GOL	2	0
3	K	203	GOL	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	140/168 (83%)	-0.06	1 (0%) 89 92	31, 47, 75, 119	0
1	B	141/168 (83%)	0.06	1 (0%) 89 92	29, 46, 74, 105	0
1	C	136/168 (80%)	0.03	0 100 100	35, 51, 73, 91	0
1	D	136/168 (80%)	-0.02	0 100 100	36, 50, 72, 85	0
1	E	137/168 (81%)	-0.04	1 (0%) 89 92	29, 46, 72, 105	0
1	F	141/168 (83%)	0.05	1 (0%) 89 92	29, 45, 74, 110	0
1	G	136/168 (80%)	0.00	0 100 100	35, 50, 70, 87	0
1	H	141/168 (83%)	0.08	3 (2%) 67 74	36, 52, 80, 114	0
1	I	136/168 (80%)	0.03	1 (0%) 89 92	36, 51, 74, 93	0
1	J	136/168 (80%)	0.01	1 (0%) 89 92	36, 50, 72, 88	0
1	K	141/168 (83%)	0.08	3 (2%) 67 74	29, 45, 73, 110	0
1	L	136/168 (80%)	-0.07	0 100 100	30, 48, 72, 95	0
All	All	1657/2016 (82%)	0.01	12 (0%) 89 92	29, 48, 74, 119	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	74	ARG	4.4
1	B	75	PRO	3.8
1	H	74	ARG	3.5
1	J	72	SER	3.4
1	K	75	PRO	3.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NA	G	201	1/1	0.94	0.21	5.31	29,29,29,29	0
2	NA	E	201	1/1	0.98	0.19	4.56	31,31,31,31	0
2	NA	A	201	1/1	0.99	0.20	4.06	34,34,34,34	0
2	NA	B	201	1/1	0.99	0.19	3.96	31,31,31,31	0
2	NA	K	201	1/1	0.94	0.21	3.83	33,33,33,33	0
2	NA	L	201	1/1	0.99	0.20	3.69	31,31,31,31	0
3	GOL	I	202	6/6	0.92	0.21	3.64	59,60,62,66	0
2	NA	F	201	1/1	0.98	0.23	3.50	31,31,31,31	0
3	GOL	D	203	6/6	0.92	0.20	3.22	63,69,69,69	0
3	GOL	B	205	6/6	0.90	0.23	3.08	79,84,85,87	0
2	NA	J	201	1/1	0.98	0.19	3.02	31,31,31,31	0
2	NA	H	201	1/1	0.99	0.17	2.54	31,31,31,31	0
3	GOL	K	203	6/6	0.89	0.19	1.85	50,59,60,62	0
3	GOL	G	202	6/6	0.95	0.15	1.83	64,67,67,67	0
3	GOL	L	202	6/6	0.94	0.16	1.57	61,62,64,65	0
3	GOL	B	203	6/6	0.87	0.17	1.53	50,55,58,58	0
3	GOL	H	202	6/6	0.96	0.17	1.48	56,58,59,63	0
2	NA	D	201	1/1	0.95	0.18	1.21	33,33,33,33	0
3	GOL	B	204	6/6	0.92	0.17	1.19	65,66,67,68	0
4	PO4	F	202	5/5	0.95	0.18	0.66	85,86,88,88	0
3	GOL	C	201	6/6	0.95	0.12	0.03	57,58,59,62	0
4	PO4	D	202	5/5	0.94	0.12	-0.08	110,110,111,111	0
4	PO4	K	202	5/5	0.96	0.15	-0.34	83,85,85,86	0
3	GOL	A	202	6/6	0.95	0.13	-0.41	53,57,58,61	0
2	NA	I	201	1/1	1.00	0.11	-0.61	31,31,31,31	0
3	GOL	J	202	6/6	0.96	0.11	-1.08	56,59,61,62	0
4	PO4	B	202	5/5	0.96	0.12	-1.32	73,75,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.