



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:22 AM GMT

PDB ID : 3EBL  
Title : Crystal Structure of Rice GID1 complexed with GA4  
Authors : Shimada, A.; Nakatsu, T.; Ueguchi-Tanaka, M.; Kato, H.; Matsuoka, M.  
Deposited on : 2008-08-28  
Resolution : 1.90 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](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

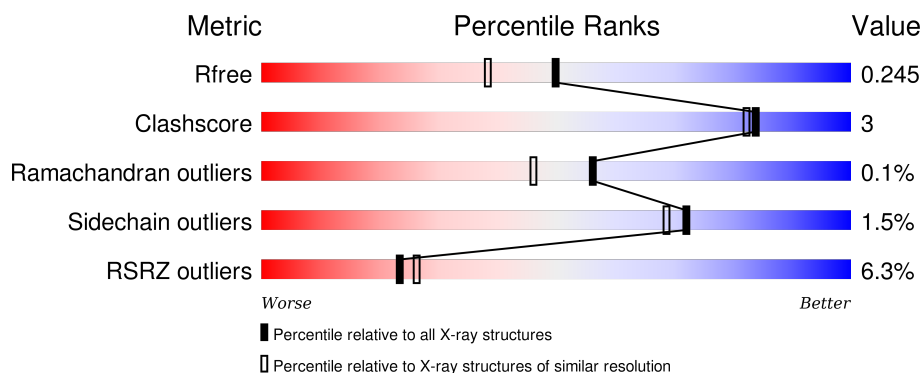
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	365	<div> <div>5%</div> <div>83%</div> <div>5%</div> <div>12%</div> </div>
1	B	365	<div> <div>5%</div> <div>82%</div> <div>5%</div> <div>13%</div> </div>
1	C	365	<div> <div>3%</div> <div>75%</div> <div>8%</div> <div>18%</div> </div>
1	D	365	<div> <div>5%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>
1	E	365	<div> <div>8%</div> <div>77%</div> <div>9%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	365	

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	MPD	B	501	-	-	-	X
3	MPD	C	501	-	-	-	X
3	MPD	D	501	-	-	-	X
3	MPD	F	501	-	-	-	X
4	NO3	A	601	-	X	-	X
4	NO3	A	602	-	X	-	X
4	NO3	A	603	-	X	-	-
4	NO3	A	604	-	X	-	X
4	NO3	B	601	-	X	-	X
4	NO3	B	602	-	X	-	X
4	NO3	B	604	-	X	-	X
4	NO3	C	601	-	X	-	X
4	NO3	C	602	-	X	-	X
4	NO3	C	603	-	X	-	X
4	NO3	C	604	-	X	-	X
4	NO3	D	601	-	X	-	-
4	NO3	D	602	-	X	-	X
4	NO3	D	603	-	X	-	-
4	NO3	E	601	-	X	-	-
4	NO3	F	601	-	X	-	X
4	NO3	F	602	-	X	-	X
4	NO3	F	603	-	X	-	-
5	PO4	E	701	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16004 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 Gibberellin receptor GID1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	5	0
			2538	1608	453	467	10			
1	B	318	Total	C	N	O	S	0	2	0
			2483	1575	442	456	10			
1	C	301	Total	C	N	O	S	0	2	0
			2360	1503	415	432	10			
1	D	315	Total	C	N	O	S	0	0	0
			2450	1561	429	450	10			
1	E	315	Total	C	N	O	S	0	2	0
			2392	1527	415	440	10			
1	F	305	Total	C	N	O	S	0	2	0
			2374	1516	414	435	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	EXPRESSION TAG	UNP Q6L545
A	356	SER	-	EXPRESSION TAG	UNP Q6L545
A	357	HIS	-	EXPRESSION TAG	UNP Q6L545
A	358	HIS	-	EXPRESSION TAG	UNP Q6L545
A	359	HIS	-	EXPRESSION TAG	UNP Q6L545
A	360	HIS	-	EXPRESSION TAG	UNP Q6L545
A	361	HIS	-	EXPRESSION TAG	UNP Q6L545
A	362	HIS	-	EXPRESSION TAG	UNP Q6L545
A	363	HIS	-	EXPRESSION TAG	UNP Q6L545
A	364	HIS	-	EXPRESSION TAG	UNP Q6L545
A	365	HIS	-	EXPRESSION TAG	UNP Q6L545
A	366	HIS	-	EXPRESSION TAG	UNP Q6L545
B	355	GLY	-	EXPRESSION TAG	UNP Q6L545
B	356	SER	-	EXPRESSION TAG	UNP Q6L545
B	357	HIS	-	EXPRESSION TAG	UNP Q6L545
B	358	HIS	-	EXPRESSION TAG	UNP Q6L545
B	359	HIS	-	EXPRESSION TAG	UNP Q6L545

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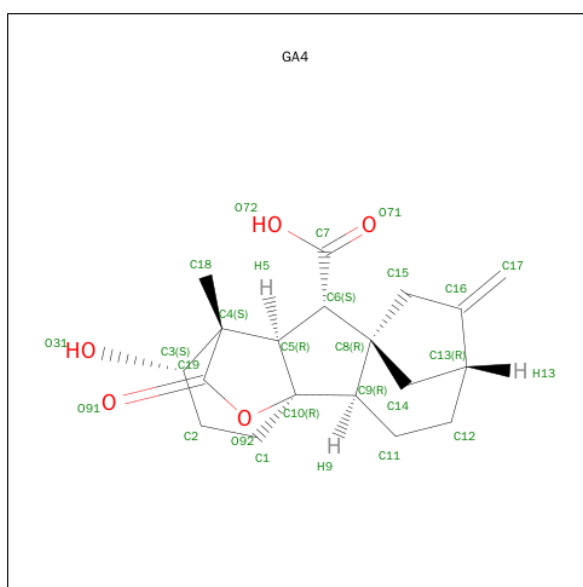
Chain	Residue	Modelled	Actual	Comment	Reference
B	360	HIS	-	EXPRESSION TAG	UNP Q6L545
B	361	HIS	-	EXPRESSION TAG	UNP Q6L545
B	362	HIS	-	EXPRESSION TAG	UNP Q6L545
B	363	HIS	-	EXPRESSION TAG	UNP Q6L545
B	364	HIS	-	EXPRESSION TAG	UNP Q6L545
B	365	HIS	-	EXPRESSION TAG	UNP Q6L545
B	366	HIS	-	EXPRESSION TAG	UNP Q6L545
C	355	GLY	-	EXPRESSION TAG	UNP Q6L545
C	356	SER	-	EXPRESSION TAG	UNP Q6L545
C	357	HIS	-	EXPRESSION TAG	UNP Q6L545
C	358	HIS	-	EXPRESSION TAG	UNP Q6L545
C	359	HIS	-	EXPRESSION TAG	UNP Q6L545
C	360	HIS	-	EXPRESSION TAG	UNP Q6L545
C	361	HIS	-	EXPRESSION TAG	UNP Q6L545
C	362	HIS	-	EXPRESSION TAG	UNP Q6L545
C	363	HIS	-	EXPRESSION TAG	UNP Q6L545
C	364	HIS	-	EXPRESSION TAG	UNP Q6L545
C	365	HIS	-	EXPRESSION TAG	UNP Q6L545
C	366	HIS	-	EXPRESSION TAG	UNP Q6L545
D	355	GLY	-	EXPRESSION TAG	UNP Q6L545
D	356	SER	-	EXPRESSION TAG	UNP Q6L545
D	357	HIS	-	EXPRESSION TAG	UNP Q6L545
D	358	HIS	-	EXPRESSION TAG	UNP Q6L545
D	359	HIS	-	EXPRESSION TAG	UNP Q6L545
D	360	HIS	-	EXPRESSION TAG	UNP Q6L545
D	361	HIS	-	EXPRESSION TAG	UNP Q6L545
D	362	HIS	-	EXPRESSION TAG	UNP Q6L545
D	363	HIS	-	EXPRESSION TAG	UNP Q6L545
D	364	HIS	-	EXPRESSION TAG	UNP Q6L545
D	365	HIS	-	EXPRESSION TAG	UNP Q6L545
D	366	HIS	-	EXPRESSION TAG	UNP Q6L545
E	355	GLY	-	EXPRESSION TAG	UNP Q6L545
E	356	SER	-	EXPRESSION TAG	UNP Q6L545
E	357	HIS	-	EXPRESSION TAG	UNP Q6L545
E	358	HIS	-	EXPRESSION TAG	UNP Q6L545
E	359	HIS	-	EXPRESSION TAG	UNP Q6L545
E	360	HIS	-	EXPRESSION TAG	UNP Q6L545
E	361	HIS	-	EXPRESSION TAG	UNP Q6L545
E	362	HIS	-	EXPRESSION TAG	UNP Q6L545
E	363	HIS	-	EXPRESSION TAG	UNP Q6L545
E	364	HIS	-	EXPRESSION TAG	UNP Q6L545
E	365	HIS	-	EXPRESSION TAG	UNP Q6L545

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Chain	Residue	Modelled	Actual	Comment	Reference
E	366	HIS	-	EXPRESSION TAG	UNP Q6L545
F	355	GLY	-	EXPRESSION TAG	UNP Q6L545
F	356	SER	-	EXPRESSION TAG	UNP Q6L545
F	357	HIS	-	EXPRESSION TAG	UNP Q6L545
F	358	HIS	-	EXPRESSION TAG	UNP Q6L545
F	359	HIS	-	EXPRESSION TAG	UNP Q6L545
F	360	HIS	-	EXPRESSION TAG	UNP Q6L545
F	361	HIS	-	EXPRESSION TAG	UNP Q6L545
F	362	HIS	-	EXPRESSION TAG	UNP Q6L545
F	363	HIS	-	EXPRESSION TAG	UNP Q6L545
F	364	HIS	-	EXPRESSION TAG	UNP Q6L545
F	365	HIS	-	EXPRESSION TAG	UNP Q6L545
F	366	HIS	-	EXPRESSION TAG	UNP Q6L545

- Molecule 2 is GIBBERELLIN A4 (three-letter code: GA4) (formula: C<sub>19</sub>H<sub>24</sub>O<sub>5</sub>).



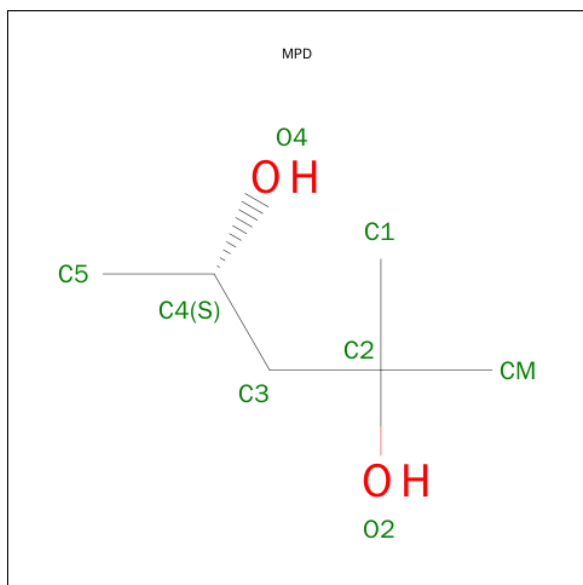
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	19	5		
2	B	1	Total	C	O	0	0
			24	19	5		
2	C	1	Total	C	O	0	0
			24	19	5		
2	D	1	Total	C	O	0	0
			24	19	5		
2	E	1	Total	C	O	0	0
			24	19	5		

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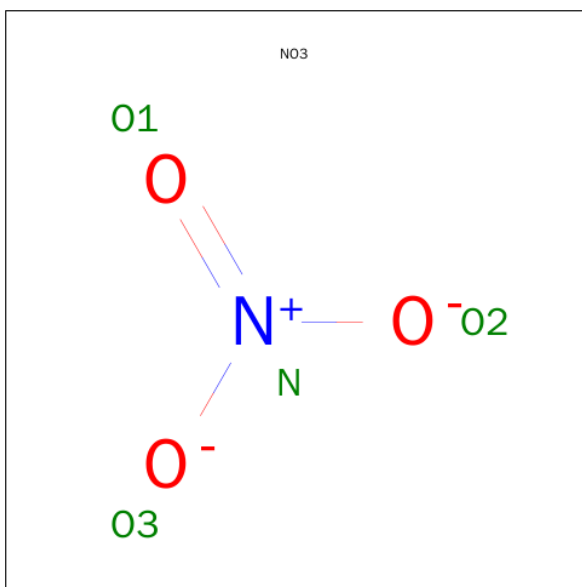
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			24	19	5		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula:  $NO_3$ ).



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

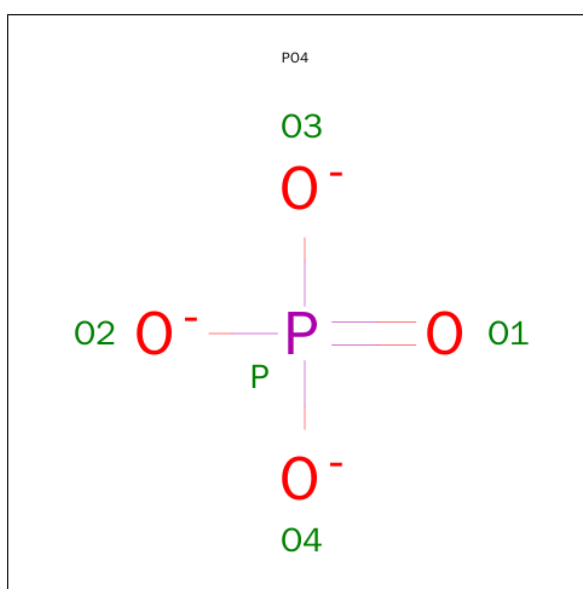
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	N	O	0	0
			4	1	3		
4	F	1	Total	N	O	0	0
			4	1	3		
4	F	1	Total	N	O	0	0
			4	1	3		
4	F	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 6 is water.

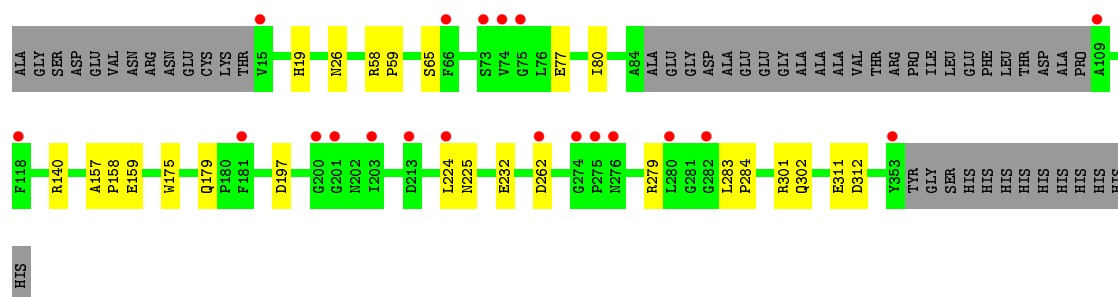
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	249	Total	O	0	0
			249	249		
6	B	204	Total	O	0	0
			204	204		
6	C	183	Total	O	0	0
			183	183		

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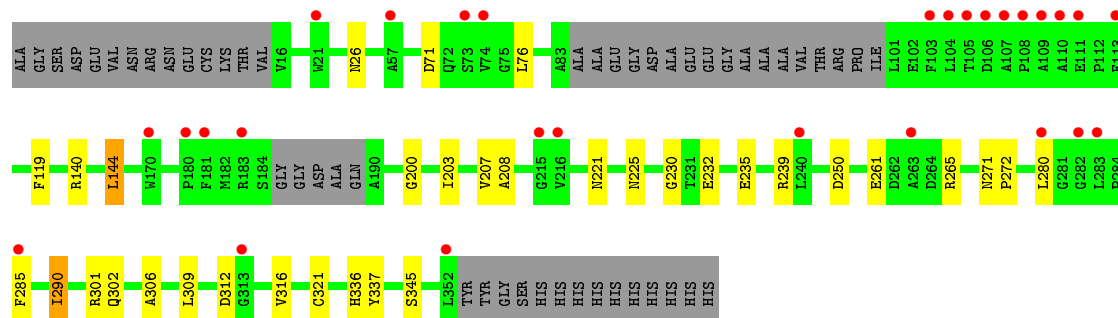
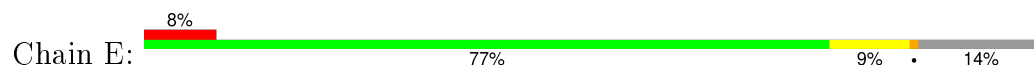
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	204	Total 204	O 204	0	0
6	E	124	Total 124	O 124	0	0
6	F	169	Total 169	O 169	0	0

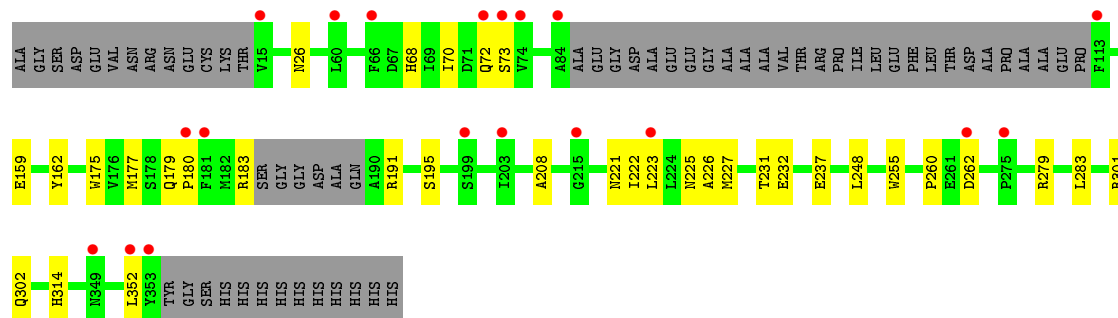
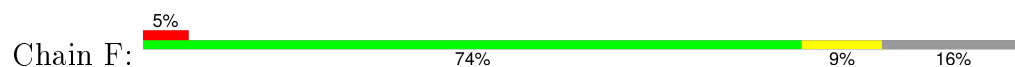




• Molecule 1: Gibberellin receptor GID1



• Molecule 1: Gibberellin receptor GID1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.76Å 133.90Å 118.89Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 35.57 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 98.7 (35.57-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.200 , 0.244 0.202 , 0.245	Depositor DCC
$R_{free}$ test set	9761 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 193845 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16004	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GA4, MPD, NO3

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	0.75	0/2630	0.73	1/3573 (0.0%)
1	B	0.72	0/2554	0.69	0/3471
1	C	0.68	0/2430	0.70	0/3301
1	D	0.70	0/2514	0.69	0/3419
1	E	0.61	0/2463	0.64	0/3359
1	F	0.66	0/2445	0.66	0/3324
All	All	0.69	0/15036	0.69	1/20447 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	LEU	CA-CB-CG	5.14	127.11	115.30

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	2538	0	2417	12	0
1	B	2483	0	2362	10	0
1	C	2360	0	2243	17	0
1	D	2450	0	2313	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2392	0	2215	19	0
1	F	2374	0	2233	17	0
2	A	24	0	23	0	0
2	B	24	0	23	0	0
2	C	24	0	23	0	0
2	D	24	0	23	0	0
2	E	24	0	23	0	0
2	F	24	0	23	0	0
3	A	8	0	14	1	0
3	B	8	0	14	1	0
3	C	8	0	14	1	0
3	D	8	0	14	1	0
3	E	8	0	14	1	0
3	F	8	0	14	1	0
4	A	16	0	0	1	0
4	B	12	0	0	0	0
4	C	16	0	0	2	0
4	D	12	0	0	0	0
4	E	4	0	0	0	0
4	F	12	0	0	1	0
5	B	5	0	0	0	0
5	E	5	0	0	0	0
6	A	249	0	0	2	0
6	B	204	0	0	0	0
6	C	183	0	0	3	0
6	D	204	0	0	0	0
6	E	124	0	0	0	0
6	F	169	0	0	0	0
All	All	16004	0	14005	88	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 3.

The worst 5 of 88 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:144:LEU:CD1	1:E:345:SER:HB2	2.15	0.77
3:E:501:MPD:H13	3:F:501:MPD:H13	1.67	0.77
1:A:26:ASN:HD22	1:B:26:ASN:HD22	1.35	0.74
1:A:231:THR:HG22	4:A:602:NO3:O3	1.92	0.70
1:F:232:GLU:O	1:F:301:ARG:NH2	2.25	0.69

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	324/365 (89%)	315 (97%)	9 (3%)	0	100	100
1	B	314/365 (86%)	300 (96%)	14 (4%)	0	100	100
1	C	297/365 (81%)	287 (97%)	9 (3%)	1 (0%)	46	35
1	D	311/365 (85%)	301 (97%)	10 (3%)	0	100	100
1	E	311/365 (85%)	297 (96%)	14 (4%)	0	100	100
1	F	301/365 (82%)	294 (98%)	6 (2%)	1 (0%)	46	35
All	All	1858/2190 (85%)	1794 (97%)	62 (3%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	286	ALA
1	F	73	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	
1	A	265/302 (88%)	263 (99%)	2 (1%)	86	86
1	B	256/302 (85%)	252 (98%)	4 (2%)	70	66
1	C	245/302 (81%)	241 (98%)	4 (2%)	70	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	248/302 (82%)	244 (98%)	4 (2%)	70	66
1	E	237/302 (78%)	233 (98%)	4 (2%)	68	64
1	F	239/302 (79%)	234 (98%)	5 (2%)	61	55
All	All	1490/1812 (82%)	1467 (98%)	23 (2%)	72	69

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	77	GLU
1	D	159	GLU
1	F	177	MET
1	D	140	ARG
1	D	262	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	221	ASN
1	E	26	ASN
1	E	221	ASN
1	D	179	GLN
1	E	206	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 ⓘ

32 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	GA4	A	401	-	25,28,28	1.14	3 (12%)	31,49,49	2.08	8 (25%)
3	MPD	A	501	-	6,7,7	0.36	0	7,10,10	0.42	0
4	NO3	A	601	-	3,3,3	3.32	3 (100%)	3,3,3	0.50	0
4	NO3	A	602	-	3,3,3	3.44	3 (100%)	3,3,3	0.22	0
4	NO3	A	603	-	3,3,3	3.47	3 (100%)	3,3,3	0.15	0
4	NO3	A	604	-	3,3,3	3.33	3 (100%)	3,3,3	0.05	0
2	GA4	B	401	-	25,28,28	1.36	3 (12%)	31,49,49	2.06	6 (19%)
3	MPD	B	501	-	6,7,7	0.33	0	7,10,10	0.48	0
4	NO3	B	601	-	3,3,3	3.47	3 (100%)	3,3,3	0.28	0
4	NO3	B	602	-	3,3,3	3.22	3 (100%)	3,3,3	0.17	0
4	NO3	B	604	-	3,3,3	3.20	3 (100%)	3,3,3	0.20	0
5	PO4	B	701	-	4,4,4	0.31	0	6,6,6	0.27	0
2	GA4	C	401	-	25,28,28	1.12	3 (12%)	31,49,49	2.23	7 (22%)
3	MPD	C	501	-	6,7,7	0.31	0	7,10,10	0.62	0
4	NO3	C	601	-	3,3,3	3.35	3 (100%)	3,3,3	0.24	0
4	NO3	C	602	-	3,3,3	3.34	3 (100%)	3,3,3	0.17	0
4	NO3	C	603	-	3,3,3	3.35	3 (100%)	3,3,3	0.22	0
4	NO3	C	604	-	3,3,3	3.19	3 (100%)	3,3,3	0.34	0
2	GA4	D	401	-	25,28,28	1.29	2 (8%)	31,49,49	1.93	5 (16%)
3	MPD	D	501	-	6,7,7	0.41	0	7,10,10	0.40	0
4	NO3	D	601	-	3,3,3	3.37	3 (100%)	3,3,3	0.23	0
4	NO3	D	602	-	3,3,3	3.35	3 (100%)	3,3,3	0.18	0
4	NO3	D	603	-	3,3,3	3.32	3 (100%)	3,3,3	0.21	0
2	GA4	E	401	-	25,28,28	1.25	2 (8%)	31,49,49	2.19	6 (19%)
3	MPD	E	501	-	6,7,7	0.28	0	7,10,10	0.41	0
4	NO3	E	601	-	3,3,3	3.31	3 (100%)	3,3,3	0.14	0
5	PO4	E	701	-	4,4,4	0.38	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GA4	F	401	-	25,28,28	1.29	2 (8%)	31,49,49	1.82	6 (19%)
3	MPD	F	501	-	6,7,7	0.22	0	7,10,10	0.44	0
4	NO3	F	601	-	3,3,3	3.40	3 (100%)	3,3,3	0.25	0
4	NO3	F	602	-	3,3,3	3.27	3 (100%)	3,3,3	0.08	0
4	NO3	F	603	-	3,3,3	3.38	3 (100%)	3,3,3	0.12	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	GA4	A	401	-	-	0/0/80/80	0/0/5/5
3	MPD	A	501	-	-	0/5/5/5	0/0/0/0
4	NO3	A	601	-	-	0/0/0/0	0/0/0/0
4	NO3	A	602	-	-	0/0/0/0	0/0/0/0
4	NO3	A	603	-	-	0/0/0/0	0/0/0/0
4	NO3	A	604	-	-	0/0/0/0	0/0/0/0
2	GA4	B	401	-	-	0/0/80/80	0/0/5/5
3	MPD	B	501	-	-	0/5/5/5	0/0/0/0
4	NO3	B	601	-	-	0/0/0/0	0/0/0/0
4	NO3	B	602	-	-	0/0/0/0	0/0/0/0
4	NO3	B	604	-	-	0/0/0/0	0/0/0/0
5	PO4	B	701	-	-	0/0/0/0	0/0/0/0
2	GA4	C	401	-	-	0/0/80/80	0/0/5/5
3	MPD	C	501	-	-	0/5/5/5	0/0/0/0
4	NO3	C	601	-	-	0/0/0/0	0/0/0/0
4	NO3	C	602	-	-	0/0/0/0	0/0/0/0
4	NO3	C	603	-	-	0/0/0/0	0/0/0/0
4	NO3	C	604	-	-	0/0/0/0	0/0/0/0
2	GA4	D	401	-	-	0/0/80/80	0/0/5/5
3	MPD	D	501	-	-	0/5/5/5	0/0/0/0
4	NO3	D	601	-	-	0/0/0/0	0/0/0/0
4	NO3	D	602	-	-	0/0/0/0	0/0/0/0
4	NO3	D	603	-	-	0/0/0/0	0/0/0/0
2	GA4	E	401	-	-	0/0/80/80	0/0/5/5
3	MPD	E	501	-	-	0/5/5/5	0/0/0/0
4	NO3	E	601	-	-	0/0/0/0	0/0/0/0
5	PO4	E	701	-	-	0/0/0/0	0/0/0/0
2	GA4	F	401	-	-	0/0/80/80	0/0/5/5
3	MPD	F	501	-	-	0/5/5/5	0/0/0/0
4	NO3	F	601	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NO3	F	602	-	-	0/0/0/0	0/0/0/0
4	NO3	F	603	-	-	0/0/0/0	0/0/0/0

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	GA4	O92-C10	-4.54	1.41	1.47
2	E	401	GA4	O92-C10	-3.21	1.43	1.47
2	B	401	GA4	O92-C10	-3.20	1.43	1.47
2	F	401	GA4	O92-C10	-2.72	1.43	1.47
2	C	401	GA4	C1-C10	2.08	1.56	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	GA4	C14-C13-C16	-5.32	97.90	102.13
2	C	401	GA4	C13-C16-C17	-4.08	121.77	126.14
2	C	401	GA4	C14-C13-C16	-4.02	98.94	102.13
2	A	401	GA4	C15-C16-C17	-3.90	121.17	126.35
2	A	401	GA4	C14-C13-C16	-3.88	99.04	102.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	MPD	1	0
4	A	602	NO3	1	0
3	B	501	MPD	1	0
3	C	501	MPD	1	0
4	C	602	NO3	1	0
4	C	604	NO3	1	0
3	D	501	MPD	1	0
3	E	501	MPD	1	0
3	F	501	MPD	1	0
4	F	602	NO3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	323/365 (88%)	0.07	20 (6%) 24 27	18, 28, 48, 64	1 (0%)
1	B	318/365 (87%)	0.19	20 (6%) 23 26	19, 31, 55, 73	0
1	C	301/365 (82%)	0.12	11 (3%) 45 49	20, 34, 52, 62	0
1	D	315/365 (86%)	0.17	20 (6%) 23 26	18, 31, 52, 61	0
1	E	315/365 (86%)	0.53	28 (8%) 12 13	24, 42, 62, 84	0
1	F	305/365 (83%)	0.24	19 (6%) 24 27	22, 35, 54, 65	0
All	All	1877/2190 (85%)	0.22	118 (6%) 23 26	18, 33, 56, 84	1 (0%)

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	ALA	9.3
1	B	107	ALA	6.8
1	E	110	ALA	5.7
1	A	105	THR	5.4
1	B	110	ALA	5.4

### 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 ⓘ

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(Å <sup>2</sup> )	Q<0.9
4	NO3	F	601	4/4	0.87	0.21	13.43	63,63,63,63	0
4	NO3	B	601	4/4	0.90	0.20	10.98	54,55,55,55	0
4	NO3	D	602	4/4	0.86	0.37	8.49	58,58,58,58	0
4	NO3	C	602	4/4	0.89	0.24	8.29	48,49,50,50	0
4	NO3	A	604	4/4	0.88	0.20	5.91	58,58,59,59	0
4	NO3	A	602	4/4	0.83	0.19	5.89	42,44,45,46	0
3	MPD	D	501	8/8	0.89	0.15	5.74	39,42,44,44	0
5	PO4	E	701	5/5	0.95	0.19	4.89	81,82,82,83	0
4	NO3	F	602	4/4	0.93	0.25	4.61	56,56,57,57	0
4	NO3	C	604	4/4	0.92	0.11	4.32	51,53,53,54	0
4	NO3	B	602	4/4	0.90	0.20	4.01	48,48,48,49	0
4	NO3	B	604	4/4	0.97	0.12	3.84	54,55,55,55	0
4	NO3	C	603	4/4	0.88	0.14	3.17	63,63,63,63	0
4	NO3	A	601	4/4	0.86	0.16	2.69	48,49,50,50	0
4	NO3	C	601	4/4	0.85	0.14	2.56	55,56,56,57	0
3	MPD	B	501	8/8	0.92	0.12	2.44	37,40,41,41	0
3	MPD	C	501	8/8	0.93	0.10	2.04	34,37,38,39	0
3	MPD	F	501	8/8	0.92	0.12	2.03	35,37,38,41	0
5	PO4	B	701	5/5	0.84	0.17	1.62	79,80,81,82	0
4	NO3	F	603	4/4	0.85	0.16	1.21	54,54,55,55	0
3	MPD	A	501	8/8	0.92	0.10	0.89	31,37,39,40	0
3	MPD	E	501	8/8	0.96	0.10	0.45	41,44,47,47	0
2	GA4	B	401	24/24	0.97	0.12	0.42	17,19,21,22	0
4	NO3	A	603	4/4	0.90	0.12	0.30	56,56,56,56	0
2	GA4	D	401	24/24	0.97	0.12	0.19	17,21,23,26	0
2	GA4	C	401	24/24	0.97	0.12	0.13	17,21,23,26	0
2	GA4	A	401	24/24	0.97	0.10	-0.09	15,18,21,24	0
2	GA4	F	401	24/24	0.96	0.12	-0.11	18,22,27,29	0
2	GA4	E	401	24/24	0.95	0.10	-0.23	26,29,31,33	0
4	NO3	D	603	4/4	0.96	0.07	-0.85	54,54,54,54	0
4	NO3	E	601	4/4	0.89	0.17	-	80,80,80,80	0
4	NO3	D	601	4/4	0.90	0.16	-	62,62,62,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.