



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2016 – 07:45 PM EDT

PDB ID : 3DZF  
Title : Crystal structure of human CD38 extracellular domain complexed with a covalent intermediate, ara-F-ribose-5'-phosphate  
Authors : Liu, Q.; Kriksunov, I.A.; Jiang, H.; Graeff, R.; Lin, H.; Lee, H.C.; Hao, Q.  
Deposited on : 2008-07-29  
Resolution : 2.01 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
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) : rb-20027674

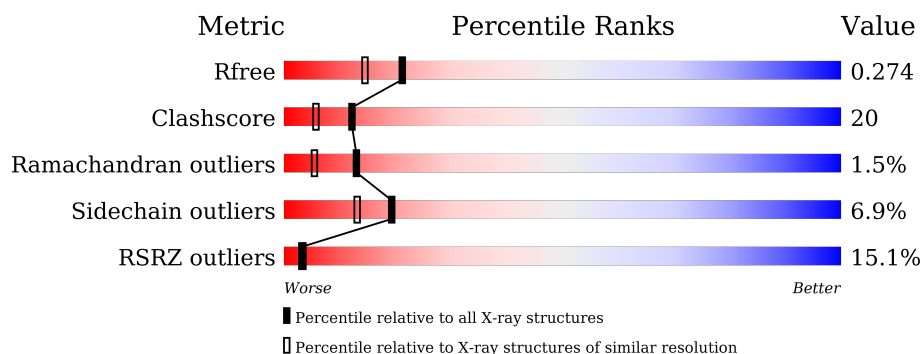
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	262	<div> <div>10%</div> <div>63%</div> <div>30%</div> <div>• •</div> </div>
1	B	262	<div> <div>9%</div> <div>65%</div> <div>29%</div> <div>• •</div> </div>
1	C	262	<div> <div>13%</div> <div>62%</div> <div>26%</div> <div>7% • •</div> </div>
1	D	262	<div> <div>24%</div> <div>59%</div> <div>32%</div> <div>5% •</div> </div>
1	E	262	<div> <div>7%</div> <div>66%</div> <div>26%</div> <div>• •</div> </div>
1	F	262	<div> <div>25%</div> <div>60%</div> <div>30%</div> <div>6% •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12987 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 ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	B	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	C	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	D	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	E	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	F	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	EXPRESSION TAG	UNP P28907
A	40	ARG	-	EXPRESSION TAG	UNP P28907
A	41	GLU	-	EXPRESSION TAG	UNP P28907
A	42	ALA	-	EXPRESSION TAG	UNP P28907
A	43	GLU	-	EXPRESSION TAG	UNP P28907
A	44	ALA	-	EXPRESSION TAG	UNP P28907
A	49	THR	GLN	ENGINEERED	UNP P28907
A	100	ASP	ASN	ENGINEERED	UNP P28907
A	164	ASP	ASN	ENGINEERED	UNP P28907
A	209	ASP	ASN	ENGINEERED	UNP P28907
A	219	ASP	ASN	ENGINEERED	UNP P28907
B	39	LYS	-	EXPRESSION TAG	UNP P28907
B	40	ARG	-	EXPRESSION TAG	UNP P28907
B	41	GLU	-	EXPRESSION TAG	UNP P28907
B	42	ALA	-	EXPRESSION TAG	UNP P28907
B	43	GLU	-	EXPRESSION TAG	UNP P28907
B	44	ALA	-	EXPRESSION TAG	UNP P28907

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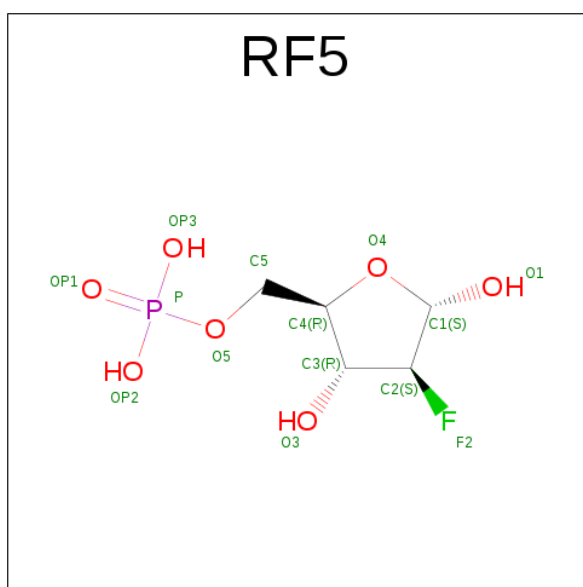
Chain	Residue	Modelled	Actual	Comment	Reference
B	49	THR	GLN	ENGINEERED	UNP P28907
B	100	ASP	ASN	ENGINEERED	UNP P28907
B	164	ASP	ASN	ENGINEERED	UNP P28907
B	209	ASP	ASN	ENGINEERED	UNP P28907
B	219	ASP	ASN	ENGINEERED	UNP P28907
C	39	LYS	-	EXPRESSION TAG	UNP P28907
C	40	ARG	-	EXPRESSION TAG	UNP P28907
C	41	GLU	-	EXPRESSION TAG	UNP P28907
C	42	ALA	-	EXPRESSION TAG	UNP P28907
C	43	GLU	-	EXPRESSION TAG	UNP P28907
C	44	ALA	-	EXPRESSION TAG	UNP P28907
C	49	THR	GLN	ENGINEERED	UNP P28907
C	100	ASP	ASN	ENGINEERED	UNP P28907
C	164	ASP	ASN	ENGINEERED	UNP P28907
C	209	ASP	ASN	ENGINEERED	UNP P28907
C	219	ASP	ASN	ENGINEERED	UNP P28907
D	39	LYS	-	EXPRESSION TAG	UNP P28907
D	40	ARG	-	EXPRESSION TAG	UNP P28907
D	41	GLU	-	EXPRESSION TAG	UNP P28907
D	42	ALA	-	EXPRESSION TAG	UNP P28907
D	43	GLU	-	EXPRESSION TAG	UNP P28907
D	44	ALA	-	EXPRESSION TAG	UNP P28907
D	49	THR	GLN	ENGINEERED	UNP P28907
D	100	ASP	ASN	ENGINEERED	UNP P28907
D	164	ASP	ASN	ENGINEERED	UNP P28907
D	209	ASP	ASN	ENGINEERED	UNP P28907
D	219	ASP	ASN	ENGINEERED	UNP P28907
E	39	LYS	-	EXPRESSION TAG	UNP P28907
E	40	ARG	-	EXPRESSION TAG	UNP P28907
E	41	GLU	-	EXPRESSION TAG	UNP P28907
E	42	ALA	-	EXPRESSION TAG	UNP P28907
E	43	GLU	-	EXPRESSION TAG	UNP P28907
E	44	ALA	-	EXPRESSION TAG	UNP P28907
E	49	THR	GLN	ENGINEERED	UNP P28907
E	100	ASP	ASN	ENGINEERED	UNP P28907
E	164	ASP	ASN	ENGINEERED	UNP P28907
E	209	ASP	ASN	ENGINEERED	UNP P28907
E	219	ASP	ASN	ENGINEERED	UNP P28907
F	39	LYS	-	EXPRESSION TAG	UNP P28907
F	40	ARG	-	EXPRESSION TAG	UNP P28907
F	41	GLU	-	EXPRESSION TAG	UNP P28907
F	42	ALA	-	EXPRESSION TAG	UNP P28907

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Chain	Residue	Modelled	Actual	Comment	Reference
F	43	GLU	-	EXPRESSION TAG	UNP P28907
F	44	ALA	-	EXPRESSION TAG	UNP P28907
F	49	THR	GLN	ENGINEERED	UNP P28907
F	100	ASP	ASN	ENGINEERED	UNP P28907
F	164	ASP	ASN	ENGINEERED	UNP P28907
F	209	ASP	ASN	ENGINEERED	UNP P28907
F	219	ASP	ASN	ENGINEERED	UNP P28907

- Molecule 2 is SUGAR (2-DEOXY-2-FLUORO-5-O-PHOSPHONO-ALPHA-D-ARABINOSE) (three-letter code: RF5) (formula: C<sub>5</sub>H<sub>10</sub>FO<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	B	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	C	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	D	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	E	1	Total	C	F	O	P	0	0
			13	5	1	6	1		
2	F	1	Total	C	F	O	P	0	0
			13	5	1	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	112	Total 112	O 112	0	0
3	C	93	Total 93	O 93	0	0
3	D	81	Total 81	O 81	0	0
3	E	115	Total 115	O 115	0	0
3	F	110	Total 110	O 110	0	0

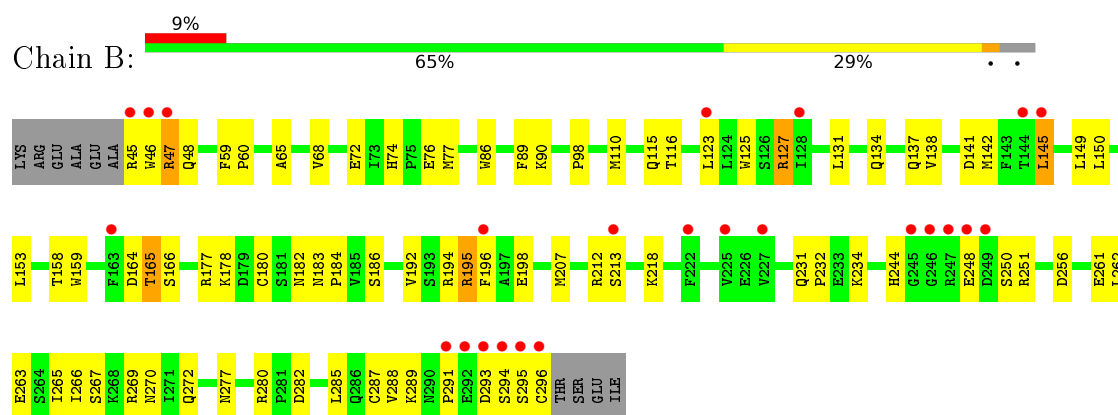
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

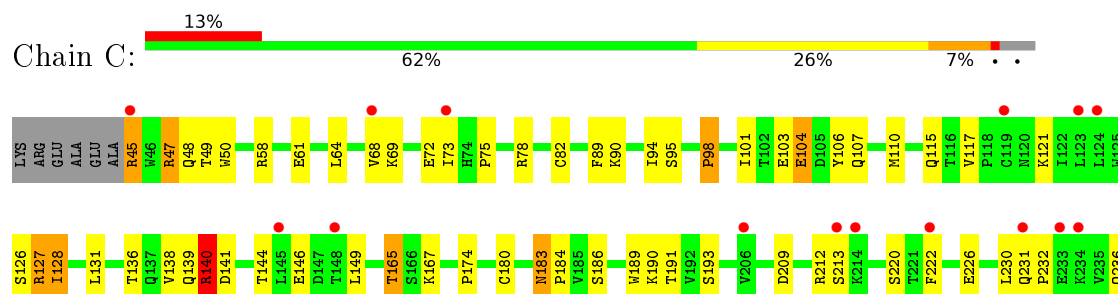
#### • Molecule 1: ADP-ribosyl cyclase 1

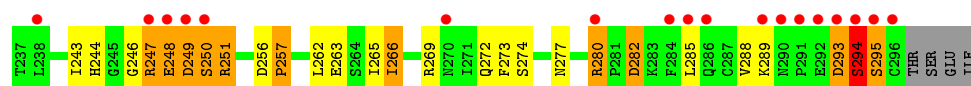


#### • Molecule 1: ADP-ribosyl cyclase 1

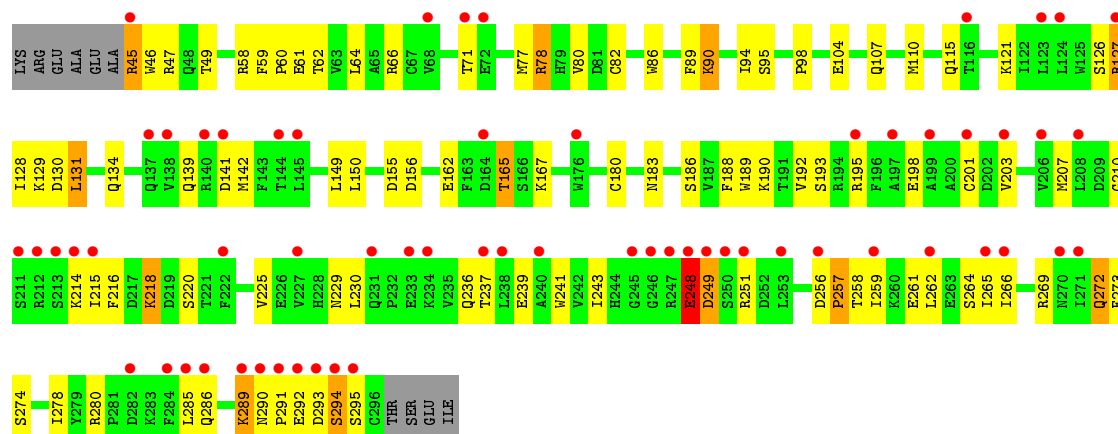


#### • Molecule 1: ADP-ribosyl cyclase 1

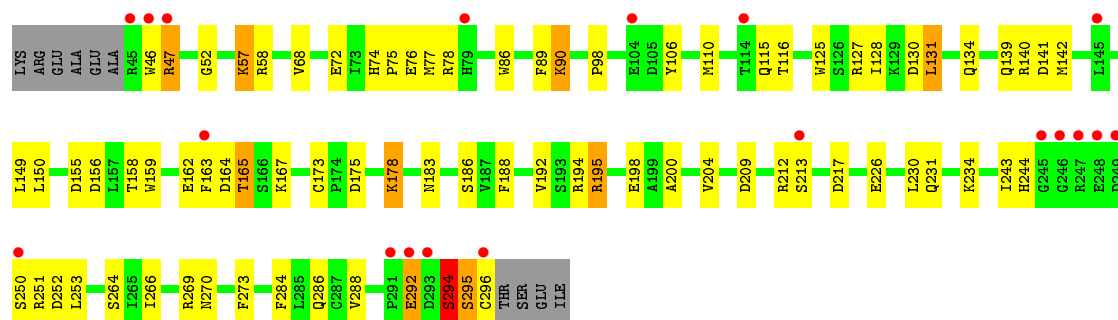




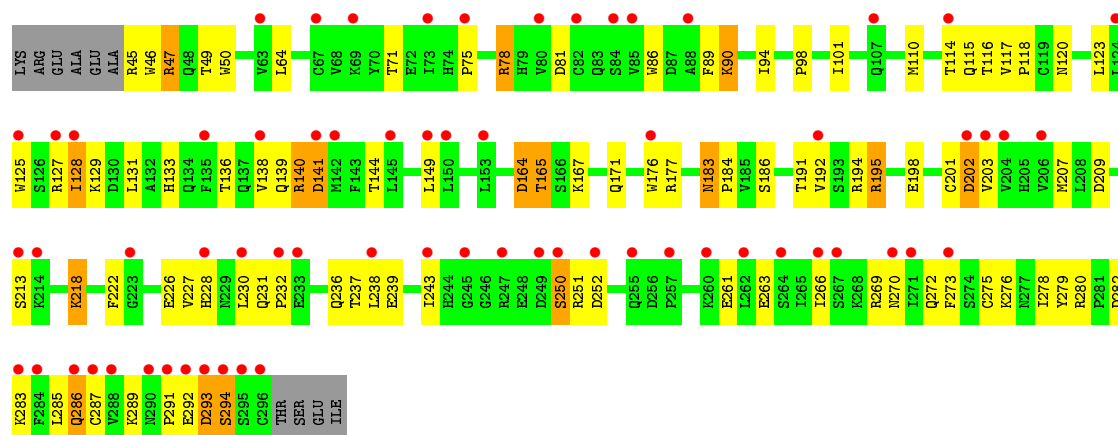
• Molecule 1: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.75Å 96.16Å 103.61Å 79.48° 82.72° 86.78°	Depositor
Resolution (Å)	20.00 – 2.01 30.11 – 2.01	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-2.01) 81.8 (30.11-2.01)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.201 , 0.272 0.203 , 0.274	Depositor DCC
$R_{free}$ test set	4493 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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 76.38 % 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 1.0517e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: RF5

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	1.11	4/2101 (0.2%)	1.00	4/2846 (0.1%)
1	B	1.11	2/2101 (0.1%)	0.98	2/2846 (0.1%)
1	C	0.95	2/2101 (0.1%)	0.92	0/2846
1	D	0.92	2/2101 (0.1%)	0.86	0/2846
1	E	1.08	0/2101	0.97	0/2846
1	F	1.01	2/2101 (0.1%)	0.92	3/2846 (0.1%)
All	All	1.03	12/12606 (0.1%)	0.94	9/17076 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	VAL	CB-CG1	6.66	1.66	1.52
1	D	248	GLU	CG-CD	5.88	1.60	1.51
1	A	187	VAL	CB-CG2	5.86	1.65	1.52
1	A	47	ARG	N-CA	5.83	1.58	1.46
1	B	125	TRP	CE3-CZ3	5.42	1.47	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	145	LEU	CB-CG-CD2	-6.10	100.62	111.00
1	A	66	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	F	251	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	131	LEU	CB-CG-CD1	5.65	120.61	111.00

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	2050	0	1976	83	0
1	B	2050	0	1976	84	0
1	C	2050	0	1976	85	0
1	D	2050	0	1976	72	0
1	E	2050	0	1976	84	0
1	F	2050	0	1976	81	0
2	A	13	0	6	1	0
2	B	13	0	6	0	0
2	C	13	0	6	5	0
2	D	13	0	6	1	0
2	E	13	0	6	3	0
2	F	13	0	6	3	0
3	A	98	0	0	7	0
3	B	112	0	0	9	0
3	C	93	0	0	5	0
3	D	81	0	0	6	0
3	E	115	0	0	9	0
3	F	110	0	0	5	0
All	All	12987	0	11892	480	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 20.

The worst 5 of 480 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:226:GLU:OE2	2:E:301:RF5:C1	1.63	1.45
1:C:226:GLU:OE2	2:C:301:RF5:C1	1.75	1.35
1:F:226:GLU:OE2	2:F:301:RF5:C1	1.74	1.34
1:A:180:CYS:HB2	3:A:397:HOH:O	1.43	1.19
1:C:47:ARG:CB	1:C:47:ARG:HH11	1.57	1.17

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	250/262 (95%)	230 (92%)	17 (7%)	3 (1%)	16	8
1	B	250/262 (95%)	233 (93%)	15 (6%)	2 (1%)	24	15
1	C	250/262 (95%)	232 (93%)	10 (4%)	8 (3%)	5	1
1	D	250/262 (95%)	235 (94%)	11 (4%)	4 (2%)	12	5
1	E	250/262 (95%)	234 (94%)	14 (6%)	2 (1%)	24	15
1	F	250/262 (95%)	234 (94%)	13 (5%)	3 (1%)	16	8
All	All	1500/1572 (95%)	1398 (93%)	80 (5%)	22 (2%)	13	5

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	248	GLU
1	B	295	SER
1	C	247	ARG
1	C	250	SER
1	C	294	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	233/241 (97%)	219 (94%)	14 (6%)	24	17
1	B	233/241 (97%)	223 (96%)	10 (4%)	35	30
1	C	233/241 (97%)	213 (91%)	20 (9%)	13	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	233/241 (97%)	216 (93%)	17 (7%)	17	11
1	E	233/241 (97%)	219 (94%)	14 (6%)	24	17
1	F	233/241 (97%)	211 (91%)	22 (9%)	11	6
All	All	1398/1446 (97%)	1301 (93%)	97 (7%)	19	13

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	294	SER
1	D	248	GLU
1	F	213	SER
1	D	49	THR
1	D	127	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	134	GLN
1	C	290	ASN
1	F	183	ASN
1	C	244	HIS
1	A	272	GLN

### 5.3.3 RNA [i](#)

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

6 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	RF5	A	301	-	13,13,14	0.86	0	16,19,21	2.31	5 (31%)
2	RF5	B	301	-	13,13,14	1.06	1 (7%)	16,19,21	2.16	7 (43%)
2	RF5	C	301	-	13,13,14	1.11	0	16,19,21	2.50	5 (31%)
2	RF5	D	301	-	13,13,14	0.62	0	16,19,21	1.88	1 (6%)
2	RF5	E	301	-	13,13,14	0.72	0	16,19,21	2.90	3 (18%)
2	RF5	F	301	-	13,13,14	0.96	0	16,19,21	1.96	5 (31%)

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	RF5	A	301	-	-	0/6/19/22	0/1/1/1
2	RF5	B	301	-	-	0/6/19/22	0/1/1/1
2	RF5	C	301	-	-	0/6/19/22	0/1/1/1
2	RF5	D	301	-	-	0/6/19/22	0/1/1/1
2	RF5	E	301	-	-	0/6/19/22	0/1/1/1
2	RF5	F	301	-	-	0/6/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	RF5	P-OP3	-2.14	1.47	1.54

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	RF5	F2-C2-C3	-4.26	104.75	108.64
2	B	301	RF5	O3-C3-C2	-3.43	102.85	112.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RF5	C1-O4-C4	-3.24	99.82	108.11
2	F	301	RF5	O5-P-OP1	-3.24	98.94	107.08
2	A	301	RF5	O4-C4-C3	-2.82	99.43	104.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RF5	1	0
2	C	301	RF5	5	0
2	D	301	RF5	1	0
2	E	301	RF5	3	0
2	F	301	RF5	3	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	252/262 (96%)	0.75	25 (9%) 9 10	28, 37, 53, 68	0
1	B	252/262 (96%)	0.66	24 (9%) 10 11	27, 36, 52, 71	0
1	C	252/262 (96%)	0.89	33 (13%) 5 5	25, 37, 50, 61	0
1	D	252/262 (96%)	1.30	62 (24%) 1 1	27, 39, 54, 57	0
1	E	252/262 (96%)	0.73	19 (7%) 17 18	28, 36, 53, 68	0
1	F	252/262 (96%)	1.36	66 (26%) 1 1	26, 37, 48, 55	0
All	All	1512/1572 (96%)	0.95	229 (15%) 3 3	25, 37, 53, 71	0

The worst 5 of 229 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	ASP	16.1
1	C	248	GLU	10.7
1	E	248	GLU	10.7
1	A	249	ASP	10.4
1	D	245	GLY	10.3

### 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(Å <sup>2</sup> )	Q<0.9
2	RF5	F	301	13/14	0.94	0.12	-1.44	43,51,54,54	0
2	RF5	D	301	13/14	0.95	0.12	-1.73	48,51,57,59	0
2	RF5	C	301	13/14	0.96	0.10	-1.74	40,45,51,55	0
2	RF5	A	301	13/14	0.97	0.07	-2.54	24,29,38,41	0
2	RF5	E	301	13/14	0.98	0.07	-2.58	23,31,37,44	0
2	RF5	B	301	13/14	0.98	0.07	-3.11	19,28,35,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.