



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 06:17 AM GMT

PDB ID : 2VA0  
Title : DIFFERENTIAL REGULATION OF THE XYLAN DEGRADING APPARATUS OF CELLVIBRIO JAPONICUS BY A NOVEL TWO COMPONENT SYSTEM  
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Deposited on : 2007-08-28  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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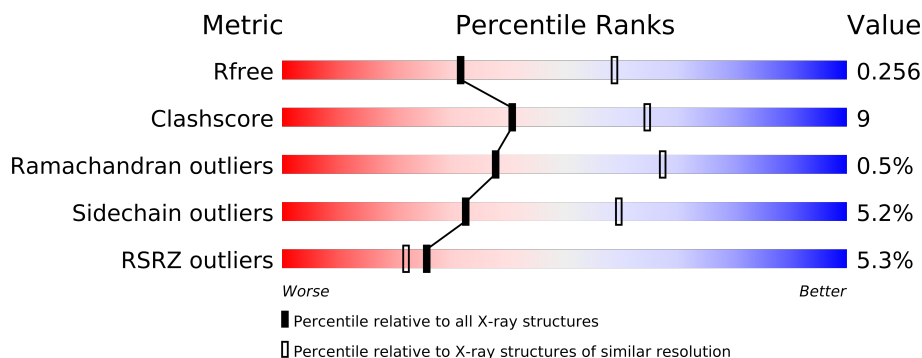
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	131	
1	B	131	
1	C	131	
1	D	131	
1	E	131	
1	F	131	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5290 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ABFS ARABINOFURANOSIDASE TWO COMPONENT SYSTEM SENSOR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			800	504	155	138	3			
1	B	119	Total	C	N	O	S	0	0	0
			973	612	182	175	4			
1	C	99	Total	C	N	O	S	0	0	0
			803	505	155	140	3			
1	D	98	Total	C	N	O	S	0	0	0
			795	501	154	137	3			
1	E	120	Total	C	N	O	S	0	0	0
			980	616	186	174	4			
1	F	99	Total	C	N	O	S	0	0	0
			800	504	155	138	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MET	-	EXPRESSION TAG	UNP B3PFT7
A	166	LEU	-	EXPRESSION TAG	UNP B3PFT7
A	167	GLU	-	EXPRESSION TAG	UNP B3PFT7
A	168	HIS	-	EXPRESSION TAG	UNP B3PFT7
A	169	HIS	-	EXPRESSION TAG	UNP B3PFT7
A	170	HIS	-	EXPRESSION TAG	UNP B3PFT7
A	171	HIS	-	EXPRESSION TAG	UNP B3PFT7
A	172	HIS	-	EXPRESSION TAG	UNP B3PFT7
A	173	HIS	-	EXPRESSION TAG	UNP B3PFT7
B	43	MET	-	EXPRESSION TAG	UNP B3PFT7
B	166	LEU	-	EXPRESSION TAG	UNP B3PFT7
B	167	GLU	-	EXPRESSION TAG	UNP B3PFT7
B	168	HIS	-	EXPRESSION TAG	UNP B3PFT7
B	169	HIS	-	EXPRESSION TAG	UNP B3PFT7
B	170	HIS	-	EXPRESSION TAG	UNP B3PFT7
B	171	HIS	-	EXPRESSION TAG	UNP B3PFT7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	172	HIS	-	EXPRESSION TAG	UNP B3PFT7
B	173	HIS	-	EXPRESSION TAG	UNP B3PFT7
C	43	MET	-	EXPRESSION TAG	UNP B3PFT7
C	166	LEU	-	EXPRESSION TAG	UNP B3PFT7
C	167	GLU	-	EXPRESSION TAG	UNP B3PFT7
C	168	HIS	-	EXPRESSION TAG	UNP B3PFT7
C	169	HIS	-	EXPRESSION TAG	UNP B3PFT7
C	170	HIS	-	EXPRESSION TAG	UNP B3PFT7
C	171	HIS	-	EXPRESSION TAG	UNP B3PFT7
C	172	HIS	-	EXPRESSION TAG	UNP B3PFT7
C	173	HIS	-	EXPRESSION TAG	UNP B3PFT7
D	43	MET	-	EXPRESSION TAG	UNP B3PFT7
D	166	LEU	-	EXPRESSION TAG	UNP B3PFT7
D	167	GLU	-	EXPRESSION TAG	UNP B3PFT7
D	168	HIS	-	EXPRESSION TAG	UNP B3PFT7
D	169	HIS	-	EXPRESSION TAG	UNP B3PFT7
D	170	HIS	-	EXPRESSION TAG	UNP B3PFT7
D	171	HIS	-	EXPRESSION TAG	UNP B3PFT7
D	172	HIS	-	EXPRESSION TAG	UNP B3PFT7
D	173	HIS	-	EXPRESSION TAG	UNP B3PFT7
E	43	MET	-	EXPRESSION TAG	UNP B3PFT7
E	166	LEU	-	EXPRESSION TAG	UNP B3PFT7
E	167	GLU	-	EXPRESSION TAG	UNP B3PFT7
E	168	HIS	-	EXPRESSION TAG	UNP B3PFT7
E	169	HIS	-	EXPRESSION TAG	UNP B3PFT7
E	170	HIS	-	EXPRESSION TAG	UNP B3PFT7
E	171	HIS	-	EXPRESSION TAG	UNP B3PFT7
E	172	HIS	-	EXPRESSION TAG	UNP B3PFT7
E	173	HIS	-	EXPRESSION TAG	UNP B3PFT7
F	43	MET	-	EXPRESSION TAG	UNP B3PFT7
F	166	LEU	-	EXPRESSION TAG	UNP B3PFT7
F	167	GLU	-	EXPRESSION TAG	UNP B3PFT7
F	168	HIS	-	EXPRESSION TAG	UNP B3PFT7
F	169	HIS	-	EXPRESSION TAG	UNP B3PFT7
F	170	HIS	-	EXPRESSION TAG	UNP B3PFT7
F	171	HIS	-	EXPRESSION TAG	UNP B3PFT7
F	172	HIS	-	EXPRESSION TAG	UNP B3PFT7
F	173	HIS	-	EXPRESSION TAG	UNP B3PFT7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

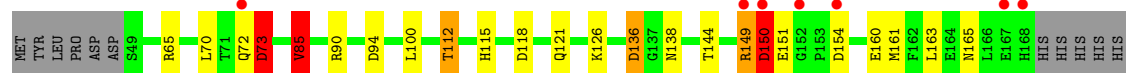
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

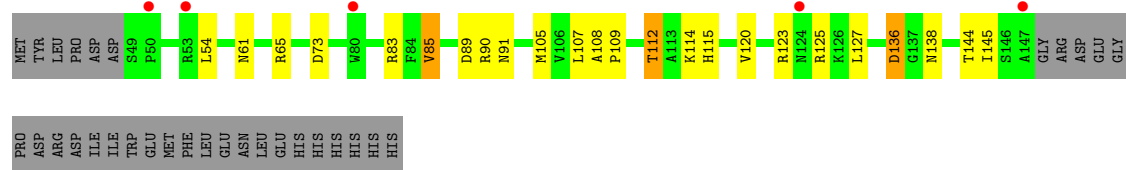
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	28	Total 28	O 28	0	0
4	C	23	Total 23	O 23	0	0
4	D	23	Total 23	O 23	0	0
4	E	11	Total 11	O 11	0	0
4	F	7	Total 7	O 7	0	0
4	D	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0
4	A	1	Total 1	O 1	0	0



Chain E: 



Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.77Å 80.01Å 101.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.04 – 2.60 37.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.04-2.60) 99.8 (37.04-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.259 0.201 , 0.256	Depositor DCC
$R_{free}$ test set	1430 reflections (5.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 2.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 27692 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.84	2/815 (0.2%)	0.96	2/1104 (0.2%)
1	B	0.91	1/992 (0.1%)	1.06	7/1343 (0.5%)
1	C	0.89	1/818 (0.1%)	1.07	5/1108 (0.5%)
1	D	0.89	1/810 (0.1%)	1.01	6/1097 (0.5%)
1	E	0.85	0/1000	1.01	4/1354 (0.3%)
1	F	0.78	0/815	0.94	3/1104 (0.3%)
All	All	0.86	5/5250 (0.1%)	1.01	27/7110 (0.4%)

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	B	0	1
1	E	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	136	ASP	CB-CG	-6.55	1.38	1.51
1	B	85	VAL	CB-CG2	-6.32	1.39	1.52
1	C	73	ASP	CB-CG	-6.22	1.38	1.51
1	A	136	ASP	CB-CG	-5.49	1.40	1.51
1	A	73	ASP	CB-CG	-5.43	1.40	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ASP	CB-CG-OD1	-8.75	110.42	118.30
1	D	136	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	C	65	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	65	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	58	MET	CG-SD-CE	-7.31	88.51	100.20
1	B	118	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C	73	ASP	CB-CA-C	6.76	123.92	110.40
1	D	65	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	85	VAL	CB-CA-C	-6.46	99.12	111.40
1	D	65	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	D	123	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	73	ASP	CB-CG-OD2	5.83	123.54	118.30
1	F	73	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	E	73	ASP	N-CA-CB	5.74	120.93	110.60
1	B	136	ASP	CB-CA-C	-5.61	99.17	110.40
1	A	136	ASP	CB-CA-C	-5.61	99.18	110.40
1	B	89	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	75	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	E	85	VAL	CB-CA-C	-5.42	101.09	111.40
1	C	85	VAL	CB-CA-C	-5.42	101.11	111.40
1	E	65	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	85	VAL	CB-CA-C	-5.23	101.46	111.40
1	D	136	ASP	CB-CA-C	-5.15	100.09	110.40
1	F	145	ILE	CB-CA-C	-5.10	101.40	111.60
1	B	73	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	F	123	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	E	136	ASP	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	47	ASP	Peptide
1	E	149	ARG	Peptide
1	E	150	ASP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	800	0	834	18	0
1	B	973	0	981	23	0
1	C	803	0	833	12	0
1	D	795	0	829	18	0
1	E	980	0	994	13	0
1	F	800	0	834	18	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
4	A	11	0	0	1	0
4	B	29	0	0	5	0
4	C	23	0	0	0	0
4	D	24	0	0	1	0
4	E	11	0	0	0	0
4	F	8	0	0	1	0
All	All	5290	0	5305	98	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (98) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:100:LEU:CD1	1:B:105:MET:CE	2.28	1.10
1:F:112:THR:HG22	1:F:115:HIS:H	1.03	1.08
1:B:100:LEU:HD13	1:B:105:MET:CE	1.85	1.07
1:D:112:THR:HG22	1:D:115:HIS:H	1.26	1.00
1:D:112:THR:HG21	2:D:1147:PO4:O1	1.61	1.00
1:B:100:LEU:CD1	1:B:105:MET:HE2	1.91	0.99
1:B:100:LEU:HD13	1:B:105:MET:HE2	1.42	0.98
1:E:112:THR:HG22	1:E:115:HIS:H	1.29	0.97
1:F:112:THR:HG21	2:F:1148:PO4:O3	1.70	0.92
1:F:112:THR:HG22	1:F:115:HIS:N	1.86	0.90
1:F:112:THR:CG2	1:F:115:HIS:H	1.87	0.86
1:B:100:LEU:CD1	1:B:105:MET:HE3	2.04	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:112:THR:HG21	2:E:1169:PO4:O3	1.77	0.84
1:B:100:LEU:HD12	1:B:105:MET:CE	2.11	0.80
1:C:112:THR:HG22	1:C:115:HIS:H	1.44	0.80
1:A:112:THR:HG22	1:A:114:LYS:H	1.47	0.78
1:C:112:THR:HG21	2:C:1147:PO4:O1	1.86	0.75
1:A:127:LEU:HG	1:A:145:ILE:HG23	1.71	0.73
1:F:112:THR:HG23	4:F:2003:HOH:O	1.90	0.72
1:F:105:MET:HA	1:F:105:MET:HE2	1.72	0.71
1:B:100:LEU:HD12	1:B:105:MET:HE2	1.70	0.69
1:D:112:THR:HG22	1:D:115:HIS:N	2.06	0.68
1:D:74:LEU:HD13	1:D:87:ILE:HD12	1.77	0.67
1:A:112:THR:HG21	2:A:1148:PO4:O3	1.96	0.66
1:E:112:THR:HG22	1:E:115:HIS:N	2.09	0.65
1:F:89:ASP:OD1	1:F:89:ASP:C	2.35	0.65
1:A:105:MET:HE1	1:A:108:ALA:HB3	1.78	0.64
1:B:112:THR:HG22	1:B:114:LYS:H	1.64	0.62
1:A:112:THR:HG22	1:A:114:LYS:N	2.14	0.62
1:F:89:ASP:OD1	1:F:91:ASN:N	2.32	0.62
1:E:150:ASP:HB3	1:E:151:GLU:HG3	1.81	0.62
1:A:105:MET:CE	1:A:108:ALA:HB3	2.30	0.61
1:F:105:MET:HA	1:F:105:MET:CE	2.30	0.60
1:B:112:THR:HG22	1:B:114:LYS:N	2.16	0.60
1:F:112:THR:HG23	1:F:114:LYS:H	1.67	0.59
1:D:108:ALA:HB3	1:D:109:PRO:HD3	1.84	0.59
1:F:54:LEU:HD21	1:F:85:VAL:HG22	1.85	0.58
1:B:100:LEU:HD12	1:B:105:MET:HE3	1.79	0.57
1:F:136:ASP:HB3	1:F:138:ASN:H	1.69	0.57
1:A:105:MET:HE2	1:A:105:MET:HA	1.86	0.56
1:F:65:ARG:HG2	1:F:65:ARG:HH11	1.71	0.55
1:B:54:LEU:HD21	1:B:85:VAL:HG22	1.90	0.54
1:D:74:LEU:HD13	1:D:87:ILE:CD1	2.38	0.54
1:B:147:ALA:N	4:B:2026:HOH:O	2.39	0.54
1:C:136:ASP:HB3	1:C:138:ASN:H	1.74	0.53
1:B:167:GLU:N	1:B:167:GLU:OE1	2.41	0.53
1:D:105:MET:HA	1:D:105:MET:HE2	1.91	0.53
1:A:105:MET:HE1	1:A:108:ALA:CB	2.39	0.52
1:B:112:THR:CG2	4:B:3002:HOH:O	2.59	0.51
1:A:107:LEU:HD13	1:A:120:VAL:HG22	1.93	0.51
1:B:164:GLU:HG2	4:B:2027:HOH:O	2.11	0.50
1:E:70:LEU:HA	1:E:73:ASP:OD1	2.12	0.50
1:D:85:VAL:HG13	1:D:144:THR:HG22	1.95	0.49
1:E:85:VAL:HG13	1:E:144:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:120:VAL:HG13	1:F:127:LEU:HB2	1.93	0.49
1:F:108:ALA:HB3	1:F:109:PRO:HD3	1.93	0.49
1:E:161:MET:O	1:E:165:ASN:HB2	2.13	0.49
1:B:112:THR:HG23	4:B:3002:HOH:O	2.12	0.49
1:E:150:ASP:HB3	1:E:151:GLU:CG	2.41	0.49
1:B:112:THR:HG21	2:B:1169:PO4:O1	2.13	0.48
1:F:112:THR:HG23	1:F:114:LYS:N	2.28	0.48
1:B:118:ASP:OD1	1:C:118:ASP:OD1	2.30	0.48
1:C:127:LEU:HD12	1:C:127:LEU:N	2.28	0.48
1:C:67:THR:OG1	1:C:136:ASP:OD2	2.19	0.48
1:D:122:ASP:OD1	1:E:115:HIS:NE2	2.47	0.47
1:B:125:ARG:HD2	4:B:2020:HOH:O	2.14	0.47
1:A:105:MET:CE	1:A:108:ALA:CB	2.93	0.46
1:A:61:ASN:HD21	1:A:65:ARG:HD2	1.80	0.46
1:B:145:ILE:HD13	1:B:145:ILE:HG21	1.56	0.46
1:C:112:THR:HG22	1:C:114:LYS:N	2.30	0.46
1:D:136:ASP:HB3	1:D:138:ASN:H	1.80	0.46
1:E:121:GLN:NE2	1:E:126:LYS:HG2	2.30	0.46
1:F:85:VAL:HG13	1:F:144:THR:HG22	1.99	0.45
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.99	0.45
1:B:112:THR:CG2	1:B:113:ALA:N	2.79	0.44
1:E:136:ASP:HB3	1:E:138:ASN:H	1.83	0.44
1:A:112:THR:CG2	1:A:113:ALA:N	2.80	0.44
1:A:74:LEU:HD23	1:A:96:LEU:HG	1.99	0.44
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.99	0.44
1:D:101:PRO:HD2	1:D:104:ILE:HG13	2.00	0.44
1:A:112:THR:CG2	4:A:3004:HOH:O	2.66	0.43
1:A:90:ARG:HH21	1:A:138:ASN:HA	1.84	0.43
1:D:118:ASP:OD1	1:E:118:ASP:OD1	2.36	0.42
1:D:49:SER:N	1:D:50:PRO:CD	2.82	0.42
1:D:120:VAL:HG12	1:D:127:LEU:HB2	2.01	0.42
1:A:121:GLN:NE2	1:A:126:LYS:HG3	2.35	0.42
1:C:112:THR:CG2	1:C:114:LYS:H	2.33	0.41
1:A:54:LEU:HD21	1:A:85:VAL:CG2	2.51	0.41
1:C:145:ILE:HG21	1:C:145:ILE:HD13	1.90	0.41
1:E:94:ASP:HB2	1:E:100:LEU:HD21	2.02	0.41
1:D:124:ASN:O	1:D:125:ARG:HG3	2.21	0.41
1:B:115:HIS:CE1	1:C:106:VAL:HG11	2.56	0.41
1:C:108:ALA:N	1:C:109:PRO:CD	2.83	0.40
1:C:112:THR:HG22	1:C:115:HIS:N	2.23	0.40
1:F:107:LEU:HD13	1:F:120:VAL:HG12	2.03	0.40
1:D:112:THR:HG23	4:D:3001:HOH:O	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:54:LEU:HD21	1:D:85:VAL:HG22	2.02	0.40
1:D:65:ARG:HH11	1:D:65:ARG:HG2	1.85	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	97/131 (74%)	95 (98%)	2 (2%)	0	100	100
1	B	115/131 (88%)	111 (96%)	4 (4%)	0	100	100
1	C	97/131 (74%)	95 (98%)	2 (2%)	0	100	100
1	D	96/131 (73%)	95 (99%)	1 (1%)	0	100	100
1	E	118/131 (90%)	114 (97%)	2 (2%)	2 (2%)	14	26
1	F	97/131 (74%)	95 (98%)	1 (1%)	1 (1%)	22	45
All	All	620/786 (79%)	605 (98%)	12 (2%)	3 (0%)	38	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	150	ASP
1	E	154	ASP
1	F	83	ARG

### 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	89/119 (75%)	85 (96%)	4 (4%)	38	67
1	B	108/119 (91%)	101 (94%)	7 (6%)	24	46
1	C	90/119 (76%)	88 (98%)	2 (2%)	64	89
1	D	89/119 (75%)	86 (97%)	3 (3%)	49	78
1	E	108/119 (91%)	100 (93%)	8 (7%)	20	38
1	F	89/119 (75%)	83 (93%)	6 (7%)	23	44
All	All	573/714 (80%)	543 (95%)	30 (5%)	32	59

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	83	ARG
1	A	120	VAL
1	A	145	ILE
1	B	47	ASP
1	B	53	ARG
1	B	85	VAL
1	B	112	THR
1	B	138	ASN
1	B	145	ILE
1	B	167	GLU
1	C	85	VAL
1	C	112	THR
1	D	85	VAL
1	D	112	THR
1	D	136	ASP
1	E	72	GLN
1	E	73	ASP
1	E	85	VAL
1	E	90	ARG
1	E	112	THR
1	E	149	ARG
1	E	160	GLU
1	E	163	LEU
1	F	61	ASN
1	F	85	VAL
1	F	90	ARG
1	F	112	THR
1	F	125	ARG
1	F	136	ASP



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	121	GLN
1	B	124	ASN
1	E	72	GLN
1	E	121	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z  > 2$
2	PO4	A	1148	-	4,4,4	0.33	0	6,6,6	0.30	0
2	PO4	B	1169	-	4,4,4	0.25	0	6,6,6	0.32	0
2	PO4	C	1147	-	4,4,4	0.51	0	6,6,6	0.32	0
2	PO4	D	1147	-	4,4,4	0.17	0	6,6,6	0.36	0
2	PO4	E	1169	-	4,4,4	0.41	0	6,6,6	0.32	0
2	PO4	F	1148	-	4,4,4	0.22	0	6,6,6	0.29	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	PO4	A	1148	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1169	-	-	0/0/0/0	0/0/0/0
2	PO4	C	1147	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1147	-	-	0/0/0/0	0/0/0/0
2	PO4	E	1169	-	-	0/0/0/0	0/0/0/0
2	PO4	F	1148	-	-	0/0/0/0	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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	99/131 (75%)	0.46	12 (12%) 5 4	3, 9, 17, 22	0
1	B	119/131 (90%)	0.25	2 (1%) 67 66	3, 9, 24, 35	0
1	C	99/131 (75%)	0.21	3 (3%) 48 45	3, 9, 19, 22	0
1	D	98/131 (74%)	0.28	5 (5%) 27 23	3, 9, 17, 22	0
1	E	120/131 (91%)	0.25	7 (5%) 22 19	3, 11, 36, 49	0
1	F	99/131 (75%)	0.14	5 (5%) 27 23	3, 9, 18, 21	0
All	All	634/786 (80%)	0.26	34 (5%) 25 21	3, 9, 22, 49	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	80	TRP	5.9
1	E	149	ARG	4.5
1	A	147	ALA	4.5
1	F	80	TRP	4.2
1	A	83	ARG	4.2
1	A	80	TRP	4.1
1	C	48	ASP	3.9
1	E	150	ASP	3.6
1	A	124	ASN	3.6
1	F	124	ASN	2.9
1	E	152	GLY	2.8
1	A	125	ARG	2.8
1	A	50	PRO	2.7
1	E	72	GLN	2.7
1	F	53	ARG	2.5
1	D	84	PHE	2.5
1	D	83	ARG	2.4
1	F	147	ALA	2.5
1	D	125	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	124	ASN	2.3
1	D	79	ASN	2.3
1	B	151	GLU	2.3
1	A	145	ILE	2.3
1	F	50	PRO	2.3
1	E	167	GLU	2.2
1	A	68	GLN	2.2
1	C	68	GLN	2.2
1	E	168	HIS	2.2
1	A	49	SER	2.1
1	A	146	SER	2.1
1	E	154	ASP	2.1
1	A	79	ASN	2.1
1	A	78	PRO	2.1
1	B	47	ASP	2.0

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	A	1148	5/5	0.13	-0.34	29,29,30,32	0
2	PO4	F	1148	5/5	0.16	-0.54	24,27,28,28	0
2	PO4	E	1169	5/5	0.12	-1.91	16,17,20,20	0
3	CL	F	1149	1/1	0.13	-1.94	8,8,8,8	0
2	PO4	C	1147	5/5	0.12	-2.37	12,12,17,17	0
2	PO4	D	1147	5/5	0.12	-2.49	7,9,13,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	C	1148	1/1	0.11	-2.65	3,3,3,3	0
2	PO4	B	1169	5/5	0.12	-2.77	14,18,21,23	0
3	CL	A	1149	1/1	0.08	-3.27	7,7,7,7	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.