



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:12 am GMT

PDB ID : 4I9E  
Title : Crystal structure of Aspartyl phosphate phosphatase F from *Bacillus subtilis*  
Authors : Marina, A.; Gallego, F.  
Deposited on : 2012-12-05  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

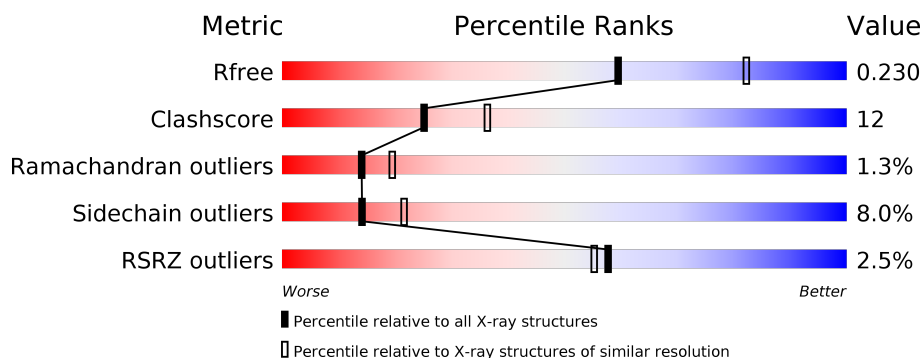
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	383	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	383	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6873 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.

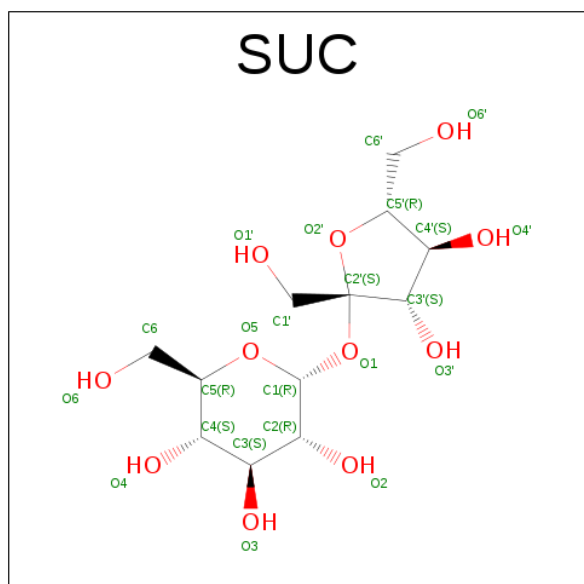
- Molecule 1 is a protein called Response regulator aspartate phosphatase F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	2	0
			3245	2106	518	605	16			
1	B	383	Total	C	N	O	S	0	6	0
			3276	2124	527	608	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P71002
A	0	ALA	-	EXPRESSION TAG	UNP P71002
B	-1	GLY	-	EXPRESSION TAG	UNP P71002
B	0	ALA	-	EXPRESSION TAG	UNP P71002

- Molecule 2 is SUGAR (SUCROSE) (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 23	C 12	O 11	0	0
2	B	1	Total 23	C 12	O 11	0	0

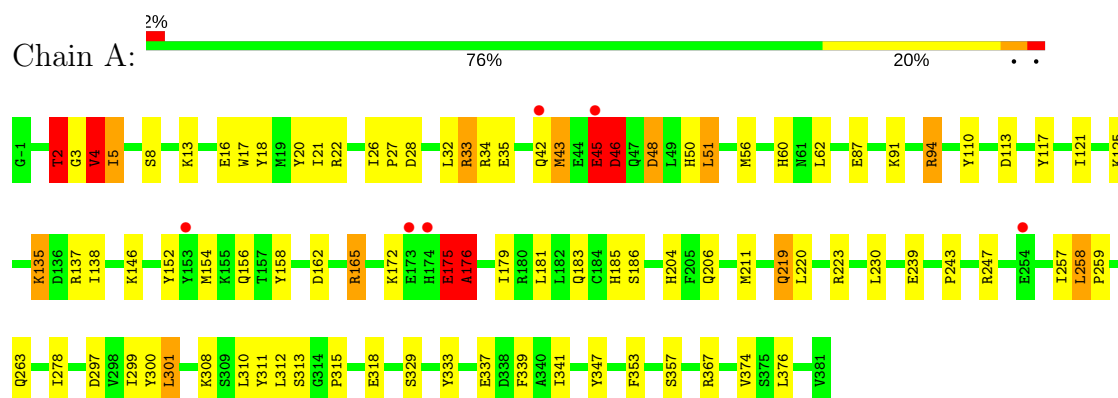
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total 174	O 174	0	0
3	B	132	Total 132	O 132	0	0

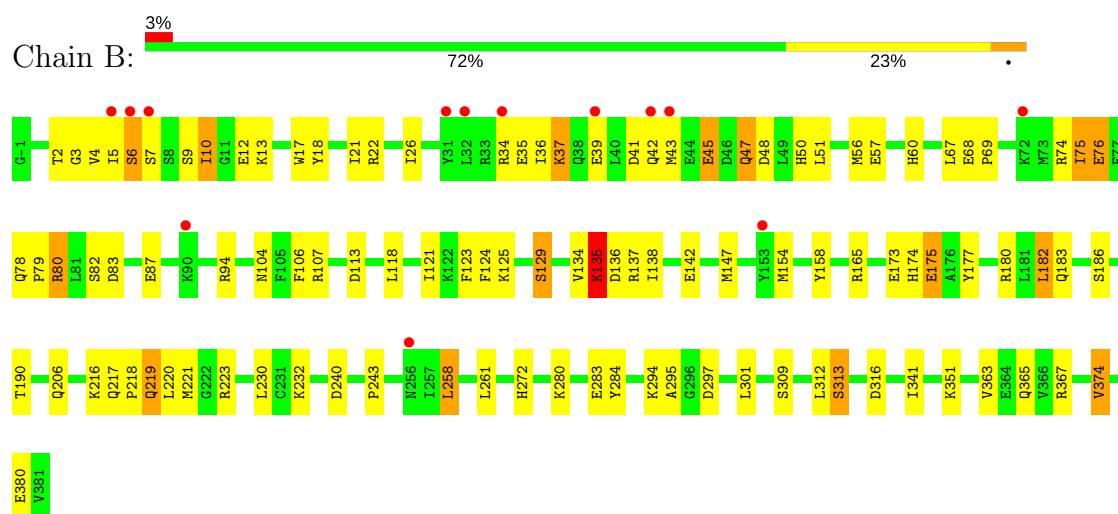
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Response regulator aspartate phosphatase F



- Molecule 1: Response regulator aspartate phosphatase F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.21Å 97.21Å 203.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.21 – 2.40 42.09 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (84.21-2.40) 99.9 (42.09-2.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.240 0.192 , 0.230	Depositor DCC
$R_{free}$ test set	2231 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6873	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.99	4/3324 (0.1%)	0.90	6/4463 (0.1%)
1	B	0.93	1/3356 (0.0%)	0.87	1/4504 (0.0%)
All	All	0.96	5/6680 (0.1%)	0.89	7/8967 (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	A	0	4
1	B	0	4
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	SER	CA-CB	9.60	1.67	1.52
1	A	318	GLU	CG-CD	6.34	1.61	1.51
1	A	239	GLU	CD-OE2	5.49	1.31	1.25
1	A	339	PHE	CE1-CZ	5.31	1.47	1.37
1	A	152	TYR	CE2-CZ	5.12	1.45	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	A	301	LEU	CA-CB-CG	5.56	128.10	115.30
1	B	129	SER	N-CA-CB	-5.54	102.19	110.50
1	A	176	ALA	CB-CA-C	5.46	118.29	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	4	VAL	N-CA-C	5.05	124.63	111.00
1	A	45	GLU	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	GLU	Peptide
1	A	176	ALA	Peptide
1	A	2	THR	Peptide
1	A	4	VAL	Peptide
1	B	134	VAL	Peptide
1	B	3	GLY	Peptide
1	B	47	GLN	Peptide
1	B	5	ILE	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	3245	0	3154	86	0
1	B	3276	0	3168	82	0
2	A	23	0	22	1	0
2	B	23	0	22	0	0
3	A	174	0	0	5	0
3	B	132	0	0	2	0
All	All	6873	0	6366	156	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 12.

All (156) 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:A:21:ILE:HD12	1:A:56:MET:HE1	1.22	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:HG3	1:A:176:ALA:H	1.14	1.09
1:A:16:GLU:OE2	3:A:660:HOH:O	1.70	1.08
1:A:21:ILE:HD12	1:A:56:MET:CE	1.85	1.06
1:A:4:VAL:HG12	1:A:5:ILE:HG23	1.35	1.06
1:A:175:GLU:CG	1:A:176:ALA:H	1.69	1.04
1:B:48:ASP:HB3	1:B:106:PHE:HZ	1.21	1.02
1:A:175:GLU:HG3	1:A:176:ALA:N	1.69	0.99
1:A:367:ARG:HE	1:B:367[B]:ARG:NH1	1.60	0.98
1:B:47:GLN:HG2	1:B:50:HIS:CD2	1.99	0.97
1:A:2:THR:HG23	1:A:3:GLY:HA2	1.50	0.94
1:B:137:ARG:NH2	1:B:173:GLU:OE2	2.05	0.88
1:A:2:THR:HG23	1:A:3:GLY:CA	2.05	0.87
1:B:47:GLN:HG2	1:B:50:HIS:HD2	1.40	0.85
1:B:17:TRP:HE1	1:B:60:HIS:HD2	1.24	0.82
1:B:10:ILE:HD12	1:B:36:ILE:HG23	1.60	0.82
1:B:48:ASP:HB3	1:B:106:PHE:CZ	2.12	0.82
1:A:158:TYR:CD2	1:B:154:MET:HE3	2.16	0.81
1:B:10:ILE:CD1	1:B:36:ILE:HG23	2.11	0.80
1:B:2:THR:C	1:B:223:ARG:HH21	1.87	0.78
1:A:4:VAL:CG1	1:A:5:ILE:HG23	2.12	0.76
1:A:87:GLU:OE1	1:A:91:LYS:HE3	1.87	0.73
1:A:337:GLU:OE2	1:A:367:ARG:NH1	2.23	0.71
1:A:46:ASP:O	1:A:50:HIS:HD2	1.74	0.70
1:B:68:GLU:HB2	1:B:69:PRO:HD3	1.72	0.70
1:A:367:ARG:NE	1:B:367[B]:ARG:NH1	2.39	0.69
1:A:17:TRP:HE1	1:A:60:HIS:HD2	1.41	0.68
1:A:263:GLN:HG3	1:A:300:TYR:OH	1.94	0.68
1:A:158:TYR:HD2	1:B:154:MET:HE3	1.59	0.68
1:B:174[B]:HIS:ND1	1:B:177:TYR:CD2	2.63	0.67
1:A:94:ARG:HD3	1:A:135:LYS:NZ	2.09	0.67
1:A:21:ILE:CD1	1:A:56:MET:CE	2.69	0.66
1:A:16:GLU:OE1	3:A:628:HOH:O	2.13	0.66
1:B:174[B]:HIS:CE1	1:B:177:TYR:HE2	2.14	0.65
1:A:315:PRO:HG2	1:A:347:TYR:OH	1.95	0.65
1:B:174[B]:HIS:HD1	1:B:177:TYR:HD2	1.45	0.64
1:B:124:PHE:HB3	1:B:147:MET:CE	2.28	0.64
1:B:78:GLN:HB2	1:B:79:PRO:HD2	1.80	0.63
1:A:185:HIS:HD2	1:A:204:HIS:ND1	1.96	0.63
1:B:47:GLN:CG	1:B:50:HIS:HD2	2.12	0.62
1:B:217:GLN:HG2	1:B:220:LEU:HD12	1.81	0.62
1:B:174[B]:HIS:ND1	1:B:177:TYR:CE2	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG12	1:A:5:ILE:CG2	2.23	0.61
1:B:45:GLU:CD	1:B:45:GLU:H	2.04	0.61
1:A:175:GLU:CG	1:A:176:ALA:N	2.37	0.60
1:B:217:GLN:HG3	3:B:520:HOH:O	2.00	0.60
1:B:219:GLN:HB3	3:B:520:HOH:O	2.01	0.60
1:A:21:ILE:HD12	1:A:56:MET:HE3	1.83	0.60
1:A:121:ILE:O	1:A:125:LYS:HG2	2.01	0.60
1:A:258:LEU:N	1:A:259:PRO:CD	2.65	0.59
1:A:333:TYR:O	1:A:337:GLU:HG3	2.02	0.59
1:A:158:TYR:HD2	1:B:154:MET:CE	2.14	0.59
1:A:154:MET:HE3	1:B:158:TYR:CD2	2.37	0.59
1:B:137:ARG:HH22	1:B:173:GLU:CD	2.06	0.59
1:A:3:GLY:N	1:A:223:ARG:NH1	2.50	0.59
1:B:43:MET:O	1:B:45:GLU:HG3	2.04	0.58
1:B:17:TRP:HE1	1:B:60:HIS:CD2	2.14	0.58
1:A:87:GLU:OE1	1:A:91:LYS:CE	2.52	0.58
1:B:341:ILE:HG13	1:B:363:VAL:HG21	1.85	0.57
1:A:46:ASP:O	1:A:50:HIS:CD2	2.57	0.57
1:A:4:VAL:HG23	1:A:223:ARG:HH22	1.69	0.57
1:B:21:ILE:HD11	1:B:60:HIS:CD2	2.40	0.56
1:A:2:THR:CG2	1:A:3:GLY:HA2	2.30	0.55
1:B:121:ILE:HD11	1:B:154:MET:HE1	1.89	0.55
1:B:21:ILE:HG13	1:B:56:MET:CE	2.36	0.55
1:B:18:TYR:O	1:B:22:ARG:HG3	2.07	0.55
1:B:313:SER:HB3	1:B:316:ASP:HB2	1.87	0.55
1:A:179:ILE:O	1:A:183:GLN:HG3	2.07	0.54
1:B:138:ILE:O	1:B:142:GLU:HG2	2.07	0.54
1:B:124:PHE:HB3	1:B:147:MET:HE1	1.89	0.53
1:A:2:THR:HG23	1:A:3:GLY:HA3	1.88	0.53
1:A:16:GLU:HG3	1:A:32:LEU:HD11	1.91	0.53
1:A:18:TYR:O	1:A:22:ARG:HG3	2.09	0.53
1:A:17:TRP:HE1	1:A:60:HIS:CD2	2.24	0.53
1:A:175:GLU:HG2	1:A:176:ALA:H	1.70	0.52
1:B:2:THR:CA	1:B:223:ARG:HH21	2.21	0.52
1:A:21:ILE:CD1	1:A:56:MET:HE3	2.37	0.52
1:B:104:ASN:HD22	1:B:123:PHE:HD1	1.55	0.52
1:B:26:ILE:HD11	1:B:67:LEU:HD12	1.91	0.52
1:A:4:VAL:CG2	1:A:223:ARG:HH22	2.23	0.52
1:A:43:MET:HG2	1:A:45:GLU:HB2	1.92	0.51
1:A:162:ASP:OD1	1:A:165:ARG:NH1	2.43	0.50
1:B:26:ILE:HD11	1:B:67:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:CE	1:B:158:TYR:HD2	2.23	0.50
1:A:20:TYR:CD2	1:A:28:ASP:HB3	2.47	0.49
1:B:12:GLU:OE2	1:B:107:ARG:NH2	2.43	0.49
1:B:258:LEU:HD12	1:B:295:ALA:HB2	1.94	0.49
1:A:219[A]:GLN:NE2	1:A:220:LEU:HG	2.27	0.49
1:B:297:ASP:O	1:B:301:LEU:HB2	2.13	0.49
1:A:367:ARG:HG2	1:A:367:ARG:HH11	1.78	0.49
1:B:363:VAL:O	1:B:367[B]:ARG:HG3	2.13	0.48
1:A:137:ARG:NH2	3:A:610:HOH:O	2.45	0.48
1:A:154:MET:CE	1:B:158:TYR:CD2	2.96	0.48
1:A:156:GLN:NE2	1:B:158:TYR:H	2.12	0.48
1:A:16:GLU:HG3	1:A:32:LEU:CD1	2.44	0.48
1:B:230:LEU:HD23	1:B:230:LEU:O	2.13	0.48
1:B:174[B]:HIS:ND1	1:B:177:TYR:HD2	2.04	0.47
1:A:158:TYR:CD2	1:B:154:MET:CE	2.90	0.47
1:B:45:GLU:HB2	1:B:47:GLN:HG3	1.97	0.47
1:A:17:TRP:CZ2	1:A:33:ARG:HB2	2.49	0.47
1:A:243:PRO:O	1:A:247:ARG:HG3	2.13	0.47
1:A:46:ASP:HB3	1:A:48:ASP:HB2	1.96	0.47
1:A:13:LYS:NZ	3:A:504:HOH:O	2.48	0.47
1:B:34:ARG:O	1:B:37:LYS:HB3	2.15	0.47
1:B:121:ILE:HD11	1:B:154:MET:CE	2.44	0.46
1:A:117:TYR:HB3	1:A:154:MET:HE3	1.98	0.46
1:A:219[B]:GLN:HE21	1:A:257:ILE:HD12	1.79	0.46
1:A:94:ARG:HD3	1:A:135:LYS:HZ1	1.80	0.46
1:A:26:ILE:HB	1:A:27:PRO:HD3	1.97	0.46
1:A:8:SER:OG	1:A:110:TYR:HA	2.16	0.46
1:A:310:LEU:HD23	1:A:311:TYR:CZ	2.50	0.46
1:A:34:ARG:NH1	1:A:35:GLU:OE2	2.49	0.46
1:B:118:LEU:HG	1:B:374:VAL:HG22	1.98	0.46
1:B:75:ILE:O	1:B:78:GLN:HG2	2.16	0.45
3:A:521:HOH:O	1:B:125:LYS:HE3	2.15	0.45
1:A:48:ASP:OD2	1:A:146:LYS:HE3	2.16	0.45
1:A:181:LEU:HB3	1:A:211:MET:HE1	1.98	0.45
1:B:9:SER:O	1:B:13:LYS:HG3	2.17	0.45
1:A:5:ILE:H	1:A:5:ILE:HG13	1.64	0.44
1:A:219[A]:GLN:HG3	1:A:219[A]:GLN:H	1.55	0.44
1:B:341:ILE:HD11	1:B:367[B]:ARG:NH2	2.32	0.44
1:B:21:ILE:HG13	1:B:56:MET:HE2	1.99	0.44
1:A:367:ARG:HE	1:B:367[B]:ARG:HH11	1.53	0.44
1:B:258:LEU:HA	1:B:261:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLN:HE22	1:B:158:TYR:H	1.65	0.44
1:B:218:PRO:HA	1:B:221:MET:HE3	2.00	0.44
1:A:353:PHE:O	1:A:357:SER:HB3	2.19	0.43
1:B:138:ILE:HA	1:B:138:ILE:HD13	1.82	0.43
1:A:3:GLY:H	1:A:223:ARG:NH1	2.16	0.43
1:A:87:GLU:CD	1:A:91:LYS:HE3	2.39	0.43
1:A:299:ILE:HG21	2:A:401:SUC:H62	2.01	0.43
1:B:272:HIS:CE1	1:B:284:TYR:CE2	3.07	0.43
1:B:182:LEU:HD11	1:B:220:LEU:HD13	2.00	0.43
1:B:218:PRO:HA	1:B:221:MET:CE	2.49	0.43
1:B:74:ARG:NH2	1:B:76:GLU:OE2	2.51	0.43
1:B:80:ARG:HB3	1:B:83:ASP:OD2	2.19	0.42
1:A:308:LYS:O	1:A:313:SER:HB3	2.19	0.42
1:A:43:MET:HB2	1:A:43:MET:HE2	1.85	0.42
1:A:172:LYS:HE2	1:A:172:LYS:HB3	1.20	0.42
1:B:186:SER:O	1:B:190:THR:HG23	2.20	0.42
1:A:310:LEU:HD23	1:A:311:TYR:CE2	2.55	0.42
1:B:174[B]:HIS:CE1	1:B:175:GLU:OE2	2.73	0.42
1:B:309:SER:HA	1:B:313:SER:HB2	2.01	0.42
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.93	0.41
1:B:174[B]:HIS:ND1	1:B:175:GLU:OE2	2.52	0.41
1:B:180:ARG:NH1	1:B:183:GLN:OE1	2.52	0.41
1:B:39:GLU:HA	1:B:42:GLN:HE21	1.85	0.41
1:A:42:GLN:O	1:A:42:GLN:HG3	2.20	0.41
1:A:94:ARG:CD	1:A:135:LYS:NZ	2.80	0.41
1:A:341:ILE:HD13	1:A:341:ILE:HA	1.91	0.41
1:A:43:MET:CG	1:A:45:GLU:HB2	2.51	0.41
1:B:240:ASP:O	1:B:243:PRO:HD2	2.20	0.40
1:B:280:LYS:O	1:B:283:GLU:HB3	2.22	0.40

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	383/383 (100%)	363 (95%)	15 (4%)	5 (1%)	14	19
1	B	387/383 (101%)	363 (94%)	18 (5%)	6 (2%)	11	15
All	All	770/766 (100%)	726 (94%)	33 (4%)	11 (1%)	14	18

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	176	ALA
1	B	4	VAL
1	B	135[A]	LYS
1	B	135[B]	LYS
1	B	7	SER
1	A	297	ASP
1	A	46	ASP
1	A	43	MET
1	B	6	SER
1	B	75	ILE

### 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	342/342 (100%)	318 (93%)	24 (7%)	18	28
1	B	342/342 (100%)	310 (91%)	32 (9%)	10	15
All	All	684/684 (100%)	628 (92%)	56 (8%)	14	20

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	5	ILE
1	A	33	ARG
1	A	45	GLU
1	A	46	ASP

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Mol	Chain	Res	Type
1	A	48	ASP
1	A	51	LEU
1	A	94	ARG
1	A	113	ASP
1	A	135	LYS
1	A	165	ARG
1	A	175	GLU
1	A	186	SER
1	A	206	GLN
1	A	219[A]	GLN
1	A	219[B]	GLN
1	A	230	LEU
1	A	258	LEU
1	A	278	ILE
1	A	301	LEU
1	A	312	LEU
1	A	329	SER
1	A	374	VAL
1	A	376	LEU
1	B	10	ILE
1	B	35	GLU
1	B	37	LYS
1	B	41	ASP
1	B	45	GLU
1	B	51	LEU
1	B	57	GLU
1	B	76	GLU
1	B	80	ARG
1	B	82	SER
1	B	87	GLU
1	B	94	ARG
1	B	113	ASP
1	B	129	SER
1	B	135[A]	LYS
1	B	135[B]	LYS
1	B	136	ASP
1	B	165	ARG
1	B	175	GLU
1	B	182	LEU
1	B	206	GLN
1	B	216	LYS
1	B	219	GLN

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Mol	Chain	Res	Type
1	B	232	LYS
1	B	258	LEU
1	B	294	LYS
1	B	312	LEU
1	B	313	SER
1	B	351	LYS
1	B	365	GLN
1	B	374	VAL
1	B	380	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	50	HIS
1	A	60	HIS
1	A	61	ASN
1	A	78	GLN
1	A	104	ASN
1	A	156	GLN
1	A	185	HIS
1	A	191	ASN
1	A	206	GLN
1	B	42	GLN
1	B	50	HIS
1	B	60	HIS
1	B	61	ASN
1	B	104	ASN
1	B	156	GLN
1	B	206	GLN
1	B	285	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

2 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	SUC	A	401	-	24,24,24	0.77	0	36,36,36	0.84	1 (2%)
2	SUC	B	401	-	24,24,24	0.68	0	36,36,36	1.22	2 (5%)

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	SUC	A	401	-	-	0/12/51/51	0/2/2/2
2	SUC	B	401	-	-	0/12/51/51	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SUC	C6-C5-C4	-2.28	107.68	113.00
2	A	401	SUC	O5-C1-C2	2.57	115.26	110.30
2	B	401	SUC	O2'-C2'-C1'	3.28	116.52	108.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SUC	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	383/383 (100%)	-0.18	6 (1%) 72 70	21, 43, 68, 89	0
1	B	383/383 (100%)	-0.09	13 (3%) 46 44	23, 48, 81, 102	0
All	All	766/766 (100%)	-0.14	19 (2%) 58 55	21, 45, 76, 102	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	GLN	7.9
1	B	43	MET	5.7
1	B	7	SER	4.4
1	B	6	SER	4.3
1	B	31	TYR	4.3
1	B	34	ARG	3.8
1	A	45	GLU	3.6
1	A	173	GLU	3.3
1	A	153[A]	TYR	3.1
1	A	42	GLN	3.0
1	B	5	ILE	2.7
1	B	90	LYS	2.3
1	A	254	GLU	2.2
1	B	39	GLU	2.1
1	B	256	ASN	2.1
1	B	72	LYS	2.1
1	B	153[A]	TYR	2.1
1	A	174	HIS	2.1
1	B	32	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SUC	A	401	23/23	0.93	0.15	-0.09	44,50,61,66	0
2	SUC	B	401	23/23	0.96	0.10	-1.04	40,47,50,57	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.