



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2017 – 05:02 PM EST

PDB ID : 5FDN  
Title : Crystal structure of phosphoenolpyruvate carboxylase from *Arabidopsis thaliana* in complex with aspartate and citrate  
Authors : Connell, M.B.; Lee, M.J.Y.; Plaxton, W.C.; Jia, Z.  
Deposited on : 2015-12-16  
Resolution : 2.20 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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-20028442

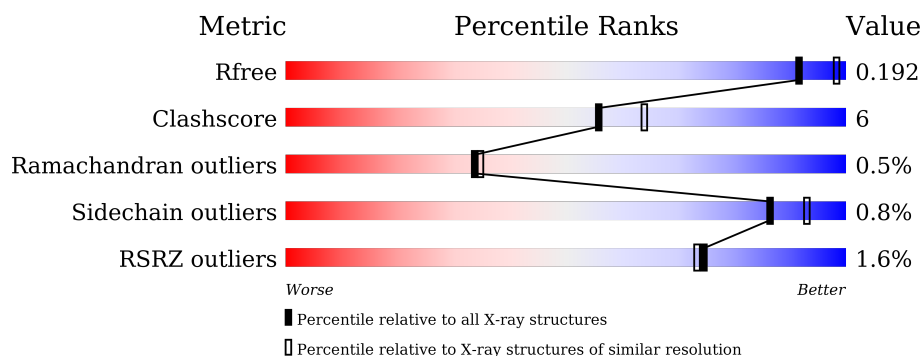
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	987	<div> <div>2%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>
1	B	987	<div> <div>%</div> <div>80%</div> <div>10%</div> <div>9%</div> </div>

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	FLC	B	1002	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16218 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 Phosphoenolpyruvate carboxylase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	914	Total	C	N	O	S	0	0	0
			7346	4659	1279	1380	28			
1	B	900	Total	C	N	O	S	0	0	0
			7227	4587	1251	1361	28			

There are 38 discrepancies between the modelled and reference sequences:

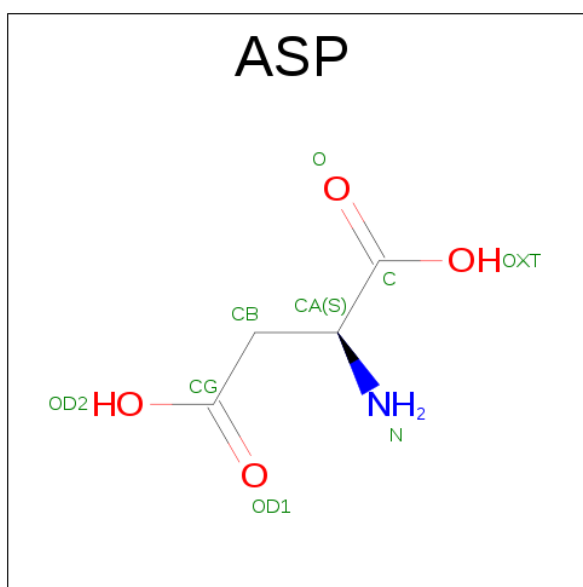
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q84VW9
A	-17	GLY	-	expression tag	UNP Q84VW9
A	-16	SER	-	expression tag	UNP Q84VW9
A	-15	SER	-	expression tag	UNP Q84VW9
A	-14	HIS	-	expression tag	UNP Q84VW9
A	-13	HIS	-	expression tag	UNP Q84VW9
A	-12	HIS	-	expression tag	UNP Q84VW9
A	-11	HIS	-	expression tag	UNP Q84VW9
A	-10	HIS	-	expression tag	UNP Q84VW9
A	-9	HIS	-	expression tag	UNP Q84VW9
A	-8	SER	-	expression tag	UNP Q84VW9
A	-7	SER	-	expression tag	UNP Q84VW9
A	-6	GLY	-	expression tag	UNP Q84VW9
A	-5	LEU	-	expression tag	UNP Q84VW9
A	-4	VAL	-	expression tag	UNP Q84VW9
A	-3	PRO	-	expression tag	UNP Q84VW9
A	-2	ARG	-	expression tag	UNP Q84VW9
A	-1	GLY	-	expression tag	UNP Q84VW9
A	0	SER	-	expression tag	UNP Q84VW9
B	-18	MET	-	initiating methionine	UNP Q84VW9
B	-17	GLY	-	expression tag	UNP Q84VW9
B	-16	SER	-	expression tag	UNP Q84VW9
B	-15	SER	-	expression tag	UNP Q84VW9
B	-14	HIS	-	expression tag	UNP Q84VW9
B	-13	HIS	-	expression tag	UNP Q84VW9

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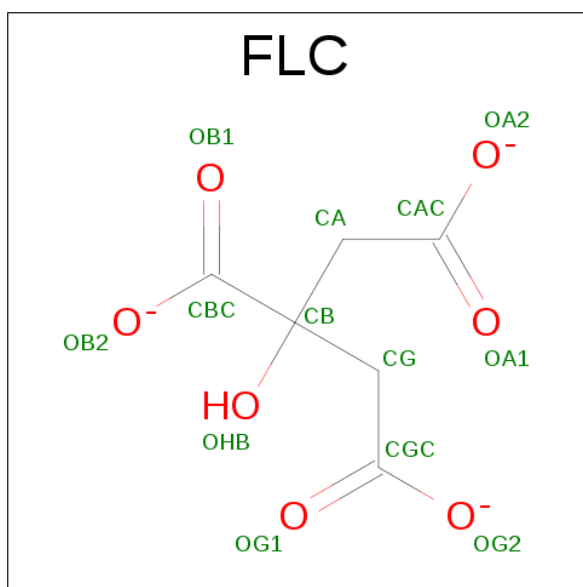
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP Q84VW9
B	-11	HIS	-	expression tag	UNP Q84VW9
B	-10	HIS	-	expression tag	UNP Q84VW9
B	-9	HIS	-	expression tag	UNP Q84VW9
B	-8	SER	-	expression tag	UNP Q84VW9
B	-7	SER	-	expression tag	UNP Q84VW9
B	-6	GLY	-	expression tag	UNP Q84VW9
B	-5	LEU	-	expression tag	UNP Q84VW9
B	-4	VAL	-	expression tag	UNP Q84VW9
B	-3	PRO	-	expression tag	UNP Q84VW9
B	-2	ARG	-	expression tag	UNP Q84VW9
B	-1	GLY	-	expression tag	UNP Q84VW9
B	0	SER	-	expression tag	UNP Q84VW9

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula:  $C_4H_7NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0

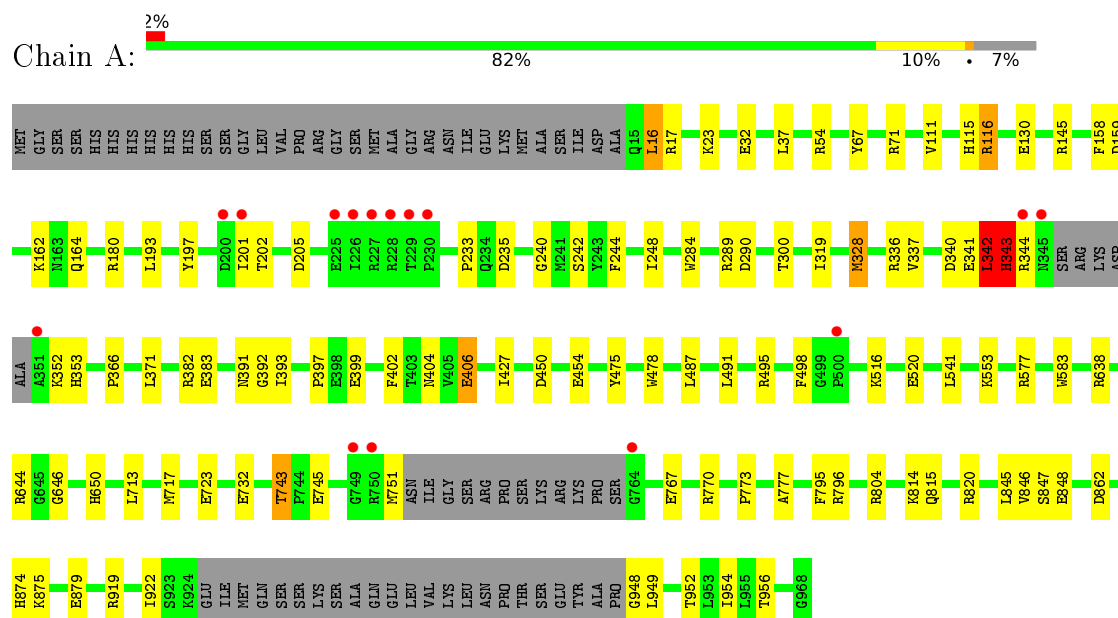
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	807	Total O 807 807	0	0
4	B	794	Total O 794 794	0	0

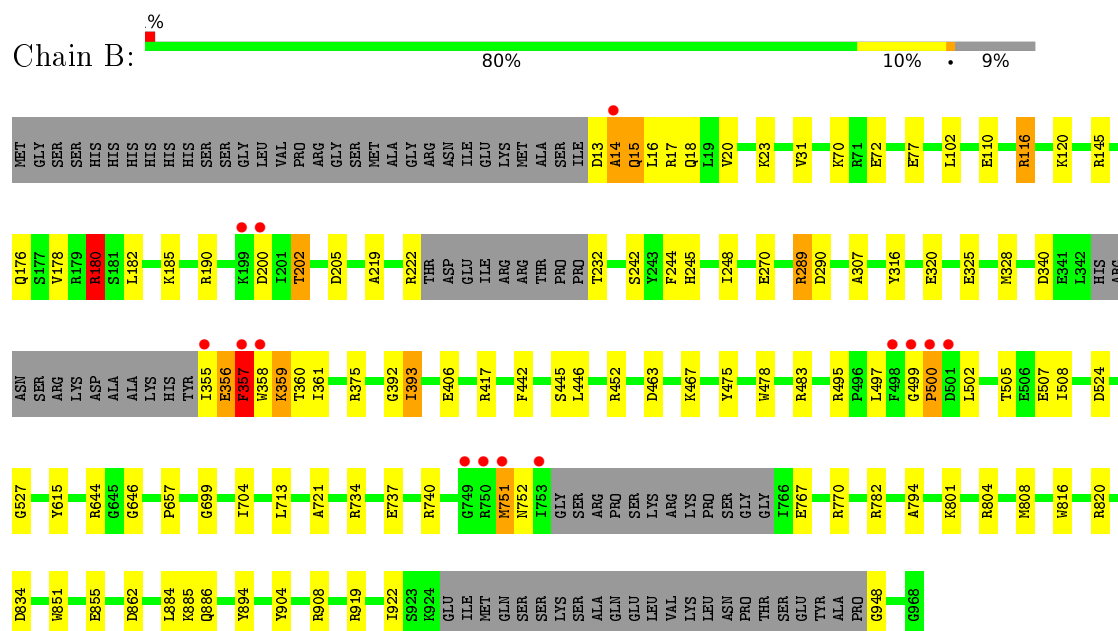
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $RSRZ > 2$ ). 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: Phosphoenolpyruvate carboxylase 3



#### • Molecule 1: Phosphoenolpyruvate carboxylase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.26 Å   268.13 Å   77.93 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.87 – 2.20 48.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.87-2.20) 99.9 (48.87-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.41 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.173 , 0.193 0.172 , 0.192	Depositor DCC
$R_{free}$ test set	2006 reflections (1.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 23.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.249 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: FLC

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	0.43	2/7498 (0.0%)	0.56	2/10146 (0.0%)
1	B	0.42	0/7373	0.61	4/9976 (0.0%)
All	All	0.42	2/14871 (0.0%)	0.58	6/20122 (0.0%)

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	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	GLU	CG-CD	7.02	1.62	1.51
1	A	406	GLU	CD-OE1	-5.62	1.19	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	180	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	B	751	MET	CA-CB-CG	6.45	124.26	113.30
1	A	116	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	751	MET	C-N-CA	5.80	136.20	121.70
1	B	116	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	342	LEU	CA-CB-CG	5.23	127.32	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	LEU	Peptide
1	A	343	HIS	Peptide
1	B	356	GLU	Peptide
1	B	699	GLY	Peptide

## 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	7346	0	7319	81	0
1	B	7227	0	7201	98	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
3	A	13	0	5	1	0
3	B	13	0	5	1	0
4	A	807	0	0	37	0
4	B	794	0	0	35	3
All	All	16218	0	14536	180	3

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 6.

All (180) 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:B:316:TYR:HH	1:B:355:ILE:N	1.41	1.19
1:B:232:THR:N	4:B:1101:HOH:O	1.84	1.09
1:B:116:ARG:NH2	4:B:1104:HOH:O	1.97	0.96
1:B:316:TYR:OH	1:B:355:ILE:N	1.99	0.96
1:A:71:ARG:N	4:A:1102:HOH:O	1.97	0.96
1:B:919:ARG:HD2	1:B:922:ILE:HD11	1.46	0.96
1:B:497:LEU:O	4:B:1102:HOH:O	1.89	0.91
1:B:14:ALA:O	1:B:16:LEU:N	2.06	0.87
1:B:245:HIS:NE2	4:B:1108:HOH:O	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ARG:O	4:B:1103:HOH:O	1.94	0.84
1:B:202:THR:HG22	1:B:205:ASP:H	1.42	0.83
1:A:948:GLY:O	4:A:1103:HOH:O	1.98	0.81
1:A:116:ARG:NH2	4:A:1108:HOH:O	2.03	0.80
1:A:919:ARG:HD2	1:A:922:ILE:HD11	1.61	0.80
1:B:804:ARG:NH1	4:B:1106:HOH:O	2.05	0.80
1:A:553:LYS:HD3	4:A:1568:HOH:O	1.83	0.79
1:A:732:GLU:OE1	4:A:1105:HOH:O	2.00	0.79
1:A:845:LEU:O	4:A:1104:HOH:O	1.98	0.78
1:A:723:GLU:OE2	4:A:1107:HOH:O	2.00	0.78
1:A:815:GLN:OE1	4:A:1106:HOH:O	2.00	0.78
1:A:804:ARG:NH1	4:A:1101:HOH:O	1.97	0.77
1:A:498:PHE:HA	4:A:1294:HOH:O	1.85	0.76
1:B:13:ASP:N	4:B:1113:HOH:O	2.17	0.76
1:A:723:GLU:HG2	4:A:1781:HOH:O	1.86	0.75
1:B:180:ARG:NH1	1:B:242:SER:HA	2.02	0.75
1:B:834:ASP:OD1	4:B:1105:HOH:O	2.04	0.75
1:B:500:PRO:HG2	1:B:502:LEU:HB2	1.67	0.75
1:B:499:GLY:H	1:B:500:PRO:HD3	1.50	0.75
1:B:15:GLN:HA	1:B:18:GLN:HG3	1.70	0.74
1:B:14:ALA:HA	1:B:17:ARG:HH11	1.54	0.72
1:B:222:ARG:O	4:B:1107:HOH:O	2.07	0.72
1:A:404:ASN:OD1	1:A:406:GLU:HB2	1.90	0.72
1:B:499:GLY:N	1:B:500:PRO:HD3	2.06	0.71
1:A:23:LYS:NZ	4:A:1119:HOH:O	2.22	0.70
1:A:202:THR:HG22	1:A:205:ASP:H	1.56	0.69
1:A:919:ARG:NH1	4:A:1109:HOH:O	2.10	0.69
1:B:885:LYS:NZ	4:B:1120:HOH:O	2.25	0.69
1:A:745:GLU:OE2	4:A:1110:HOH:O	2.12	0.67
1:B:908:ARG:O	4:B:1109:HOH:O	2.12	0.67
1:A:16:LEU:HD23	1:A:17:ARG:H	1.60	0.67
1:B:200:ASP:O	4:B:1111:HOH:O	2.12	0.67
1:B:417:ARG:NH2	4:B:1116:HOH:O	2.21	0.66
1:A:879:GLU:OE1	4:A:1112:HOH:O	2.14	0.66
1:A:862:ASP:HB2	4:A:1675:HOH:O	1.95	0.66
1:A:848:GLU:OE1	4:A:1111:HOH:O	2.13	0.66
1:B:751:MET:HB2	1:B:752:ASN:CA	2.25	0.66
1:B:524:ASP:OD2	4:B:1110:HOH:O	2.12	0.65
1:A:644:ARG:O	4:A:1113:HOH:O	2.15	0.64
1:B:948:GLY:O	4:B:1112:HOH:O	2.13	0.64
1:A:202:THR:HB	4:A:1188:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLU:O	1:A:342:LEU:HB2	1.97	0.64
1:B:245:HIS:CE1	4:B:1108:HOH:O	2.47	0.62
1:B:358:TRP:HE1	1:B:361:ILE:HG12	1.63	0.62
1:B:505:THR:HG21	4:B:1807:HOH:O	1.98	0.62
1:A:337:VAL:O	1:A:341:GLU:HG2	2.00	0.61
1:B:392:GLY:O	1:B:393:ILE:HG13	2.00	0.61
1:B:751:MET:HB2	1:B:752:ASN:HA	1.84	0.60
1:A:235:ASP:OD1	4:A:1114:HOH:O	2.17	0.59
1:A:495:ARG:NH2	4:A:1130:HOH:O	2.34	0.59
1:A:289:ARG:NH2	1:A:300:THR:OG1	2.32	0.58
1:B:355:ILE:HG23	1:B:356:GLU:HG3	1.86	0.58
1:A:116:ARG:HG2	4:A:1493:HOH:O	2.02	0.58
1:B:20:VAL:HG11	1:B:886:GLN:HG3	1.84	0.58
1:B:77:GLU:OE2	1:B:904:TYR:OH	2.22	0.57
1:B:340:ASP:OD2	4:B:1114:HOH:O	2.18	0.57
1:A:402:PHE:O	4:A:1115:HOH:O	2.17	0.57
1:A:796:ARG:NH2	4:A:1136:HOH:O	2.38	0.56
1:B:505:THR:CG2	1:B:508:ILE:H	2.18	0.56
1:B:851:TRP:O	1:B:855:GLU:HG3	2.05	0.56
1:A:180:ARG:HG3	1:A:242:SER:HB3	1.88	0.56
1:A:743:THR:HG22	1:A:745:GLU:H	1.70	0.55
1:B:70:LYS:HD3	1:B:72:GLU:CG	2.37	0.55
1:B:14:ALA:HA	1:B:17:ARG:NH1	2.21	0.55
1:A:577:ARG:NE	4:A:1143:HOH:O	2.40	0.54
1:A:159:ASP:OD2	4:A:1116:HOH:O	2.18	0.54
1:A:32:GLU:HG3	4:A:1710:HOH:O	2.07	0.54
1:B:290:ASP:O	1:B:770:ARG:NH2	2.35	0.53
1:B:180:ARG:CZ	1:B:242:SER:HA	2.37	0.53
1:B:442:PHE:HB3	1:B:446:LEU:HD23	1.91	0.52
1:B:713:LEU:HD22	1:B:808:MET:CE	2.40	0.52
1:B:289:ARG:HG3	1:B:452:ARG:O	2.11	0.51
1:B:358:TRP:O	1:B:359:LYS:HE2	2.11	0.51
1:B:704:ILE:HD11	1:B:816:TRP:HA	1.93	0.51
1:A:743:THR:CG2	1:A:777:ALA:HB1	2.41	0.51
1:A:770:ARG:HB2	1:A:773:PRO:HD2	1.93	0.51
1:B:646:GLY:N	4:B:1142:HOH:O	2.42	0.51
1:A:820:ARG:HD3	4:A:1204:HOH:O	2.10	0.51
1:B:358:TRP:CB	1:B:375:ARG:HH12	2.24	0.51
1:A:516:LYS:NZ	1:A:520:GLU:OE2	2.37	0.50
1:B:358:TRP:HB2	1:B:375:ARG:HH12	1.76	0.50
1:B:178:VAL:HG13	1:B:182:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:ARG:HG2	4:B:1816:HOH:O	2.10	0.50
1:A:638:ARG:NH1	4:A:1131:HOH:O	2.35	0.50
1:A:874:HIS:CE1	4:A:1137:HOH:O	2.64	0.50
1:B:176:GLN:O	1:B:176:GLN:HG3	2.12	0.49
1:B:23:LYS:NZ	4:B:1147:HOH:O	2.45	0.49
1:B:820:ARG:HD3	4:B:1298:HOH:O	2.12	0.49
3:A:1002:FLC:OA1	3:A:1002:FLC:OHB	2.27	0.49
1:A:717:MET:HE1	1:A:795:PHE:CD1	2.48	0.48
1:A:751:MET:HG2	1:A:954:ILE:HD11	1.93	0.48
1:B:782:ARG:NH2	4:B:1148:HOH:O	2.45	0.48
1:A:240:GLY:O	4:A:1117:HOH:O	2.20	0.48
1:B:15:GLN:NE2	4:B:1113:HOH:O	2.29	0.48
1:A:743:THR:CG2	1:A:745:GLU:H	2.26	0.48
1:B:505:THR:HG22	1:B:508:ILE:HB	1.96	0.47
1:B:180:ARG:NH1	4:B:1129:HOH:O	2.36	0.47
1:A:111:VAL:O	1:A:115:HIS:HD2	1.97	0.47
1:A:340:ASP:O	1:A:343:HIS:HB2	2.16	0.46
1:B:751:MET:HB2	1:B:752:ASN:HB2	1.97	0.46
1:A:382:ARG:NH1	1:A:383:GLU:OE2	2.49	0.45
1:B:445:SER:O	1:B:446:LEU:HB2	2.16	0.45
1:A:952:THR:O	1:A:956:THR:HG23	2.16	0.45
1:B:180:ARG:CZ	1:B:242:SER:CA	2.93	0.45
1:B:505:THR:HG23	1:B:508:ILE:H	1.80	0.45
1:B:615:TYR:CD2	1:B:657:PRO:HG3	2.52	0.45
1:A:284:TRP:CD1	1:A:450:ASP:HB2	2.52	0.45
1:B:320:GLU:OE1	1:B:357:PHE:HB3	2.17	0.45
1:A:319:ILE:HD11	1:A:371:LEU:HD22	1.99	0.45
1:B:767:GLU:CD	1:B:767:GLU:H	2.20	0.45
1:B:734:ARG:HD2	1:B:737:GLU:OE1	2.16	0.45
1:B:202:THR:HG23	4:B:1523:HOH:O	2.16	0.44
1:A:391:ASN:O	1:A:393:ILE:N	2.50	0.44
1:A:767:GLU:H	1:A:767:GLU:CD	2.21	0.44
1:B:325:GLU:OE1	4:B:1115:HOH:O	2.20	0.44
1:B:475:TYR:HA	1:B:478:TRP:CE3	2.52	0.44
1:B:307:ALA:HB1	1:B:445:SER:O	2.18	0.44
1:A:353:HIS:NE2	4:A:1129:HOH:O	2.33	0.44
1:A:244:PHE:HA	1:A:248:ILE:HB	2.00	0.43
1:B:499:GLY:N	1:B:500:PRO:CD	2.80	0.43
1:A:197:TYR:HB2	4:A:1513:HOH:O	2.18	0.43
1:A:814:LYS:HA	1:A:820:ARG:HH21	1.84	0.43
1:A:158:PHE:CE2	1:A:162:LYS:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:MET:HE2	1:A:427:ILE:HD13	2.00	0.43
1:A:130:GLU:O	1:A:650:HIS:HB3	2.18	0.43
1:A:487:LEU:HD13	1:A:541:LEU:HB2	2.01	0.43
1:A:67:TYR:O	1:A:71:ARG:N	2.50	0.43
1:A:336:ARG:NH1	1:A:366:PRO:HG3	2.34	0.43
1:B:102:LEU:HG	1:B:894:TYR:HB2	2.01	0.43
1:A:397:PRO:HB2	1:A:399:GLU:OE1	2.18	0.43
1:A:743:THR:HG21	1:A:777:ALA:HB1	2.00	0.43
1:A:713:LEU:O	1:A:717:MET:HG3	2.18	0.43
1:B:740:ARG:NH2	4:B:1160:HOH:O	2.51	0.43
1:B:721:ALA:HB2	1:B:794:ALA:HB2	2.01	0.42
1:B:862:ASP:HB2	4:B:1646:HOH:O	2.19	0.42
1:A:145:ARG:HD2	4:A:1439:HOH:O	2.18	0.42
1:B:704:ILE:H	1:B:704:ILE:HG13	1.72	0.42
1:A:201:ILE:O	1:A:201:ILE:HG22	2.19	0.42
1:A:475:TYR:HA	1:A:478:TRP:CE3	2.55	0.42
1:B:500:PRO:C	1:B:502:LEU:H	2.22	0.42
1:B:751:MET:HB2	1:B:752:ASN:CB	2.50	0.42
1:B:884:LEU:HB2	3:B:1002:FLC:OA2	2.20	0.42
1:B:527:GLY:HA3	4:B:1191:HOH:O	2.18	0.42
1:A:491:LEU:HD22	1:A:583:TRP:CZ2	2.54	0.42
1:B:145:ARG:HD2	4:B:1645:HOH:O	2.20	0.42
1:B:185:LYS:HE3	1:B:219:ALA:HB1	2.01	0.42
1:B:475:TYR:CZ	1:B:483:ARG:HD3	2.55	0.42
1:B:495:ARG:HD2	4:B:1613:HOH:O	2.19	0.42
1:B:704:ILE:O	1:B:704:ILE:HD12	2.19	0.42
1:B:801:LYS:NZ	4:B:1161:HOH:O	2.51	0.42
1:A:949:LEU:HA	4:A:1103:HOH:O	2.19	0.42
1:B:244:PHE:HA	1:B:248:ILE:HB	2.01	0.42
1:B:110:GLU:OE1	1:B:190:ARG:HD3	2.20	0.41
1:A:646:GLY:N	4:A:1165:HOH:O	2.52	0.41
1:A:393:ILE:HG13	1:A:393:ILE:O	2.19	0.41
1:A:846:VAL:HG12	1:A:847:SER:O	2.20	0.41
1:A:875:LYS:N	1:A:875:LYS:HD3	2.34	0.41
1:B:120:LYS:HA	1:B:120:LYS:HD3	1.78	0.41
1:B:15:GLN:HG2	4:B:1113:HOH:O	2.19	0.41
1:A:399:GLU:H	1:A:399:GLU:CD	2.24	0.41
1:B:270:GLU:OE2	4:B:1117:HOH:O	2.21	0.41
1:A:233:PRO:HB3	4:A:1770:HOH:O	2.20	0.41
1:B:17:ARG:HG2	1:B:31:VAL:HG11	2.03	0.41
1:A:37:LEU:HD11	1:A:193:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:THR:HG23	1:A:777:ALA:HB1	2.02	0.41
1:B:713:LEU:HD22	1:B:808:MET:HE2	2.03	0.41
1:A:290:ASP:OD1	1:A:454:GLU:HG3	2.20	0.41
1:B:70:LYS:HE2	1:B:72:GLU:HG2	2.03	0.40
1:B:463:ASP:O	1:B:467:LYS:HB2	2.21	0.40
1:B:505:THR:HG23	1:B:507:GLU:N	2.36	0.40
1:B:713:LEU:HD22	1:B:808:MET:HE3	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1731:HOH:O	4:B:1735:HOH:O[4_566]	1.83	0.37
4:B:1253:HOH:O	4:B:1592:HOH:O[1_554]	2.08	0.12
4:B:1759:HOH:O	4:B:1799:HOH:O[4_566]	2.18	0.02

## 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	906/987 (92%)	879 (97%)	24 (3%)	3 (0%)	46	50
1	B	890/987 (90%)	858 (96%)	26 (3%)	6 (1%)	26	25
All	All	1796/1974 (91%)	1737 (97%)	50 (3%)	9 (0%)	34	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	ARG
1	B	14	ALA
1	B	15	GLN
1	B	360	THR

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Mol	Chain	Res	Type
1	B	393	ILE
1	B	357	PHE
1	B	500	PRO
1	A	352	LYS
1	A	392	GLY

### 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	798/860 (93%)	792 (99%)	6 (1%)	86	93
1	B	786/860 (91%)	779 (99%)	7 (1%)	84	92
All	All	1584/1720 (92%)	1571 (99%)	13 (1%)	86	93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	164	GLN
1	A	328	MET
1	A	342	LEU
1	A	343	HIS
1	A	743	THR
1	B	180	ARG
1	B	202	THR
1	B	289	ARG
1	B	328	MET
1	B	357	PHE
1	B	359	LYS
1	B	406	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	184	GLN
1	A	245	HIS
1	A	915	ASN
1	B	245	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 ⓘ

4 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	ASP	A	1001	-	2,8,8	0.39	0	1,10,10	0.00	0
3	FLC	A	1002	-	3,12,12	1.10	0	3,17,17	5.86	3 (100%)
2	ASP	B	1001	-	2,8,8	0.35	0	1,10,10	0.06	0
3	FLC	B	1002	-	3,12,12	1.16	0	3,17,17	4.57	1 (33%)

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	ASP	A	1001	-	-	0/2/8/8	0/0/0/0
3	FLC	A	1002	-	-	0/6/16/16	0/0/0/0
2	ASP	B	1001	-	-	0/2/8/8	0/0/0/0
3	FLC	B	1002	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	FLC	CB-CA-CAC	-9.64	99.89	114.95
3	B	1002	FLC	CB-CA-CAC	-7.70	102.91	114.95
3	A	1002	FLC	CB-CG-CGC	-2.45	111.12	114.95
3	A	1002	FLC	CG-CB-CA	2.03	114.89	109.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	FLC	1	0
3	B	1002	FLC	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	914/987 (92%)	-0.60	15 (1%) 74 73	11, 24, 50, 100	0
1	B	900/987 (91%)	-0.64	14 (1%) 74 73	10, 24, 48, 72	0
All	All	1814/1974 (91%)	-0.62	29 (1%) 74 73	10, 24, 49, 100	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ILE	9.1
1	A	201	ILE	7.3
1	A	200	ASP	5.2
1	A	228	ARG	5.1
1	B	501	ASP	5.0
1	A	345	ASN	4.9
1	A	227	ARG	4.8
1	A	500	PRO	3.9
1	B	358	TRP	3.6
1	A	344	ARG	3.5
1	B	357	PHE	3.3
1	A	230	PRO	3.3
1	B	499	GLY	3.2
1	A	764	GLY	3.1
1	B	498	PHE	3.1
1	A	225	GLU	3.0
1	B	500	PRO	3.0
1	A	229	THR	3.0
1	B	749	GLY	2.8
1	B	355	ILE	2.7
1	A	351	ALA	2.6
1	B	199	LYS	2.6
1	A	750	ARG	2.4
1	A	749	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	200	ASP	2.3
1	B	750	ARG	2.2
1	B	753	ILE	2.2
1	B	751	MET	2.0
1	B	14	ALA	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(Å <sup>2</sup> )	Q<0.9
3	FLC	B	1002	13/13	0.94	0.14	2.61	18,23,35,46	0
3	FLC	A	1002	13/13	0.93	0.11	0.69	16,26,34,46	0
2	ASP	B	1001	9/9	0.96	0.09	-0.36	18,21,24,24	0
2	ASP	A	1001	9/9	0.98	0.08	-0.55	16,21,22,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.