



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:52 PM UTC

PDB ID : 4XAE / pdb\_00004xae  
Title : Structure of Feruloyl-CoA 6-hydroxylase (F6H) from Arabidopsis thaliana  
Authors : Zhou, D.; Kandavelu, P.; Zhang, H.; Wang, B.C.; Rose, J.; Yan, Y.  
Deposited on : 2014-12-14  
Resolution : 2.77 Å(reported)

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

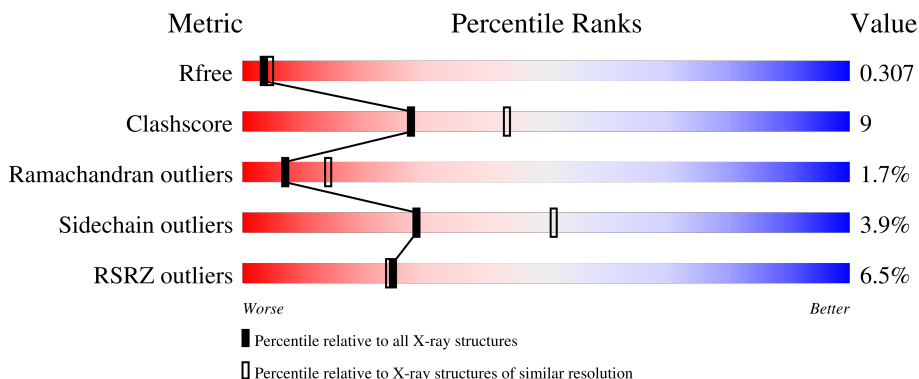
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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))
$R_{free}$	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	373	
1	B	373	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5171 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 Feruloyl CoA ortho-hydroxylase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	329	2596	1664	434	490	3	5	0	0	0
1	B	324	2545	1632	426	479	3	5	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLY	-	expression tag	UNP Q9LHN8
A	-10	SER	-	expression tag	UNP Q9LHN8
A	-9	SER	-	expression tag	UNP Q9LHN8
A	-8	HIS	-	expression tag	UNP Q9LHN8
A	-7	HIS	-	expression tag	UNP Q9LHN8
A	-6	HIS	-	expression tag	UNP Q9LHN8
A	-5	HIS	-	expression tag	UNP Q9LHN8
A	-4	HIS	-	expression tag	UNP Q9LHN8
A	-3	HIS	-	expression tag	UNP Q9LHN8
A	-2	SER	-	expression tag	UNP Q9LHN8
A	-1	GLN	-	expression tag	UNP Q9LHN8
A	0	ASP	-	expression tag	UNP Q9LHN8
A	1	PRO	-	expression tag	UNP Q9LHN8
B	-11	GLY	-	expression tag	UNP Q9LHN8
B	-10	SER	-	expression tag	UNP Q9LHN8
B	-9	SER	-	expression tag	UNP Q9LHN8
B	-8	HIS	-	expression tag	UNP Q9LHN8
B	-7	HIS	-	expression tag	UNP Q9LHN8
B	-6	HIS	-	expression tag	UNP Q9LHN8
B	-5	HIS	-	expression tag	UNP Q9LHN8
B	-4	HIS	-	expression tag	UNP Q9LHN8
B	-3	HIS	-	expression tag	UNP Q9LHN8
B	-2	SER	-	expression tag	UNP Q9LHN8
B	-1	GLN	-	expression tag	UNP Q9LHN8
B	0	ASP	-	expression tag	UNP Q9LHN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	PRO	-	expression tag	UNP Q9LHN8

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

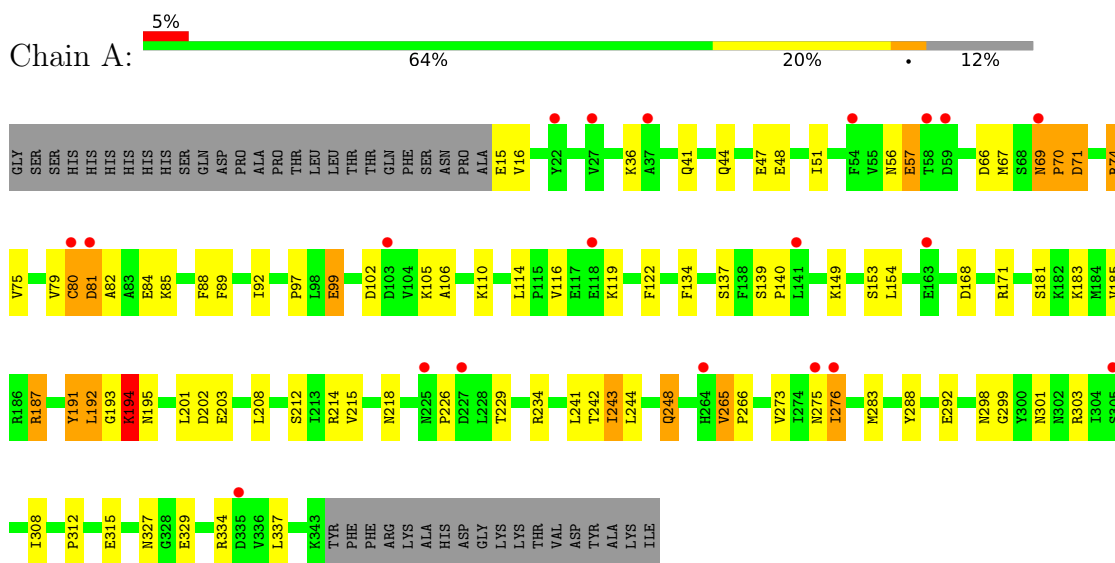
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	12	Total O 12 12	0	0

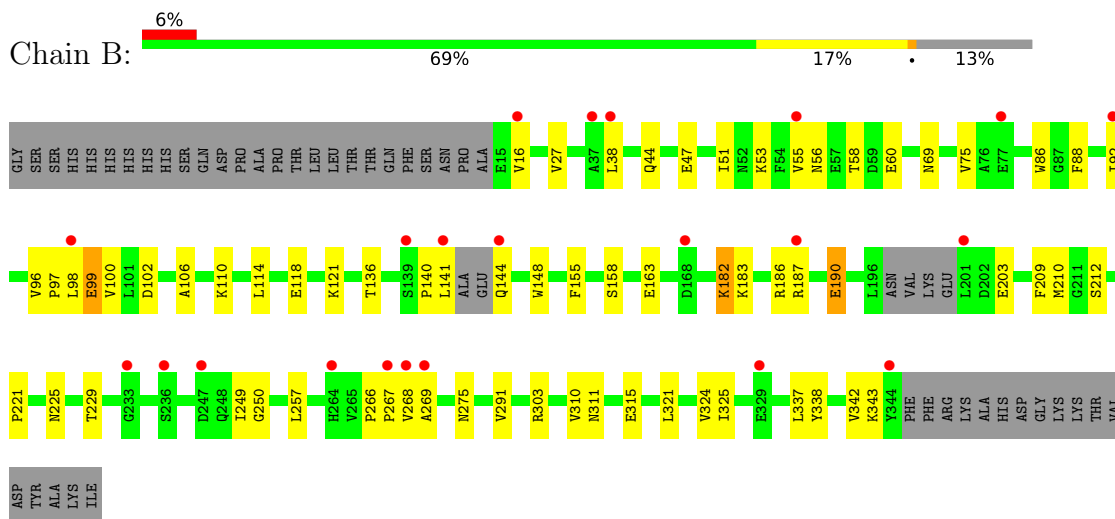
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Feruloyl CoA ortho-hydroxylase 1



- Molecule 1: Feruloyl CoA ortho-hydroxylase 1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.22Å 54.55Å 78.81Å 90.00° 111.54° 90.00°	Depositor
Resolution (Å)	44.93 – 2.77 44.93 – 2.77	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.93-2.77) 90.0 (44.93-2.77)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.243 , 0.300 0.252 , 0.307	Depositor DCC
$R_{free}$ test set	1874 reflections (9.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtrriage
Anisotropy	0.688	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.030 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: NA

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	0.50	0/2650	0.99	7/3593 (0.2%)
1	B	0.41	0/2597	0.92	13/3521 (0.4%)
All	All	0.46	0/5247	0.95	20/7114 (0.3%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	N-CA-C	-13.84	96.53	113.41
1	A	16	VAL	N-CA-C	-7.23	102.76	113.39
1	B	69	ASN	CA-C-N	6.72	126.23	119.24
1	B	69	ASN	C-N-CA	6.72	126.23	119.24
1	A	80	CYS	CA-CB-SG	-6.61	99.21	114.40
1	B	266	PRO	CA-C-N	6.49	125.93	118.85
1	B	266	PRO	C-N-CA	6.49	125.93	118.85
1	A	69	ASN	CA-C-N	6.41	127.86	119.84
1	A	69	ASN	C-N-CA	6.41	127.86	119.84
1	A	265	VAL	CA-C-N	6.41	126.98	120.38
1	A	265	VAL	C-N-CA	6.41	126.98	120.38
1	B	225	ASN	CA-C-N	6.25	125.93	119.56
1	B	225	ASN	C-N-CA	6.25	125.93	119.56
1	B	136	THR	N-CA-C	-5.57	100.61	109.07
1	B	98	LEU	CA-C-N	-5.28	114.30	122.49
1	B	98	LEU	C-N-CA	-5.28	114.30	122.49
1	B	325	ILE	N-CA-C	-5.22	107.66	112.83
1	B	96	VAL	CA-C-N	5.11	125.40	119.93
1	B	96	VAL	C-N-CA	5.11	125.40	119.93
1	B	98	LEU	N-CA-C	5.10	118.60	112.38

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	2596	0	2568	62	1
1	B	2545	0	2504	30	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	0	9	0
3	B	12	0	0	1	0
All	All	5171	0	5072	92	1

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 9.

All (92) 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:194:LYS:NZ	1:A:288:TYR:OH	2.14	0.79
1:A:194:LYS:CE	1:A:195:ASN:H	1.96	0.78
1:A:275:ASN:O	1:A:276:ILE:HG12	1.83	0.78
1:B:92:ILE:O	3:B:501:HOH:O	2.01	0.78
1:B:118:GLU:OE2	1:B:121:LYS:NZ	2.16	0.78
1:A:303:ARG:NE	3:A:505:HOH:O	2.18	0.76
1:B:257:LEU:HD11	1:B:291:VAL:HG11	1.69	0.75
1:A:194:LYS:HE3	1:A:195:ASN:H	1.53	0.72
1:A:168:ASP:OD1	1:A:171:ARG:NH2	2.22	0.71
1:A:56:ASN:OD1	1:A:57:GLU:N	2.26	0.69
1:A:84:GLU:OE2	3:A:502:HOH:O	2.11	0.69
1:A:234:ARG:HH11	1:A:234:ARG:HG3	1.59	0.68
1:A:15:GLU:OE2	3:A:503:HOH:O	2.14	0.64
1:A:244:LEU:HB3	1:A:273:VAL:HB	1.79	0.63
1:A:194:LYS:HE3	1:A:195:ASN:HD22	1.64	0.63
1:A:191:TYR:O	1:A:193:GLY:N	2.32	0.62
1:A:80:CYS:SG	1:A:194:LYS:HD3	2.40	0.61
1:B:182:LYS:HG3	1:B:210:MSE:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:CG	1:A:203:GLU:H	2.09	0.60
1:B:60:GLU:HG2	1:B:86:TRP:HH2	1.66	0.60
1:A:194:LYS:HE2	1:A:195:ASN:H	1.65	0.59
1:B:44:GLN:HG2	1:B:229:THR:HA	1.82	0.59
1:B:58:THR:HG23	1:B:60:GLU:HB2	1.85	0.59
1:B:88:PHE:CE2	1:B:275:ASN:HB3	2.38	0.58
1:A:41:GLN:OE1	3:A:504:HOH:O	2.17	0.58
1:B:47:GLU:O	1:B:51:ILE:HG13	2.03	0.58
1:A:191:TYR:O	1:A:194:LYS:HG3	2.03	0.58
1:B:186:ARG:O	1:B:190:GLU:HG2	2.03	0.58
1:B:99:GLU:HG3	1:B:102:ASP:HB2	1.87	0.57
1:A:106:ALA:O	1:A:110:LYS:HG3	2.06	0.56
1:A:102:ASP:O	3:A:501:HOH:O	2.18	0.55
1:A:242:THR:O	1:A:243:ILE:HB	2.07	0.55
1:B:97:PRO:HB2	1:B:100:VAL:HG23	1.91	0.52
1:B:56:ASN:OD1	1:B:58:THR:HG22	2.09	0.52
1:B:250:GLY:HA3	1:B:267:PRO:HB3	1.92	0.52
1:A:153:SER:HG	1:A:214:ARG:HE	1.59	0.50
1:A:298:ASN:OD1	1:A:301:ASN:N	2.34	0.50
1:A:102:ASP:C	3:A:501:HOH:O	2.53	0.50
1:A:194:LYS:HE3	1:A:195:ASN:ND2	2.25	0.50
1:A:244:LEU:N	1:A:273:VAL:O	2.41	0.50
1:A:154:LEU:HB2	1:A:215:VAL:HG13	1.93	0.50
1:A:56:ASN:CG	1:A:57:GLU:H	2.20	0.49
1:B:106:ALA:O	1:B:110:LYS:HG3	2.13	0.49
1:A:226:PRO:HG3	1:A:299:GLY:HA3	1.95	0.49
1:A:122:PHE:O	1:A:134:PHE:N	2.34	0.49
1:B:183:LYS:O	1:B:187:ARG:HG2	2.12	0.48
1:A:71:ASP:HB3	1:A:74:ARG:CZ	2.43	0.48
1:B:315:GLU:HA	1:B:337:LEU:HD11	1.94	0.48
1:B:110:LYS:O	1:B:114:LEU:HG	2.14	0.48
1:A:97:PRO:HB2	1:A:99:GLU:CG	2.44	0.47
1:A:105:LYS:N	3:A:501:HOH:O	2.47	0.47
1:A:44:GLN:HG2	1:A:229:THR:HA	1.97	0.47
1:A:202:ASP:CG	1:A:203:GLU:N	2.73	0.47
1:A:106:ALA:N	3:A:501:HOH:O	2.05	0.46
1:A:88:PHE:CE2	1:A:275:ASN:HB3	2.51	0.46
1:B:321:LEU:HB2	1:B:324:VAL:HG23	1.96	0.46
1:A:67:MSE:HB3	1:A:187:ARG:NH2	2.31	0.46
1:A:149:LYS:NZ	1:A:218:ASN:OD1	2.49	0.46
1:A:327:ASN:HB2	1:A:329:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:CZ	1:B:212:SER:HB2	2.51	0.46
1:A:139:SER:HA	1:A:140:PRO:HD3	1.86	0.45
1:A:212:SER:OG	1:A:312:PRO:O	2.30	0.45
1:A:82:ALA:HB1	1:A:89:PHE:HB3	1.99	0.45
1:A:48:GLU:HG2	1:A:234:ARG:NH1	2.32	0.45
1:A:15:GLU:CG	3:A:503:HOH:O	2.64	0.44
1:A:47:GLU:O	1:A:51:ILE:HG13	2.17	0.44
1:A:69:ASN:HA	1:A:70:PRO:HD3	1.84	0.44
1:B:148:TRP:NE1	1:B:221:PRO:HG2	2.33	0.44
1:A:80:CYS:SG	1:A:192:LEU:HD23	2.58	0.44
1:B:249:ILE:HG21	1:B:303:ARG:HD2	2.00	0.44
1:A:79:VAL:O	1:A:82:ALA:HB3	2.18	0.44
1:A:226:PRO:HG3	1:A:299:GLY:CA	2.48	0.44
1:A:248:GLN:H	1:A:248:GLN:CD	2.25	0.44
1:B:141:LEU:HD13	1:B:144:GLN:OE1	2.19	0.43
1:A:114:LEU:O	1:A:119:LYS:HE2	2.19	0.43
1:A:315:GLU:OE1	1:A:315:GLU:N	2.48	0.43
1:A:265:VAL:HA	1:A:266:PRO:HD2	1.89	0.43
1:A:315:GLU:HA	1:A:337:LEU:HD11	2.01	0.43
1:B:27:VAL:HG23	1:B:221:PRO:HG3	2.01	0.42
1:B:183:LYS:HB2	1:B:183:LYS:HE2	1.72	0.42
1:A:208:LEU:O	1:A:283:MSE:HE1	2.19	0.42
1:B:38:LEU:HD21	1:B:229:THR:HB	2.02	0.42
1:A:181:SER:O	1:A:185:VAL:HG23	2.20	0.41
1:B:338:TYR:O	1:B:342:VAL:HG23	2.19	0.41
1:A:116:VAL:HA	1:A:119:LYS:HG3	2.02	0.41
1:B:209:PHE:O	1:B:310:VAL:HG12	2.20	0.41
1:A:81:ASP:O	1:A:85:LYS:HE3	2.20	0.41
1:A:66:ASP:HB2	1:A:92:ILE:HD11	2.02	0.41
1:B:212:SER:OG	1:B:311:ASN:HB2	2.21	0.41
1:A:194:LYS:HE3	1:A:194:LYS:HB2	1.68	0.40
1:B:187:ARG:HG2	1:B:187:ARG:H	1.72	0.40
1:A:242:THR:O	1:A:308:ILE:O	2.39	0.40

All (1) 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)
1:A:201:LEU:O	1:B:203:GLU:OE2[4_555]	2.01	0.19

## 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	327/373 (88%)	306 (94%)	13 (4%)	8 (2%)	4	9
1	B	318/373 (85%)	304 (96%)	11 (4%)	3 (1%)	14	28
All	All	645/746 (86%)	610 (95%)	24 (4%)	11 (2%)	7	14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	LEU
1	A	194	LYS
1	A	276	ILE
1	B	269	ALA
1	A	70	PRO
1	A	71	ASP
1	A	191	TYR
1	A	243	ILE
1	B	140	PRO
1	A	137	SER
1	B	343	LYS

### 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	287/325 (88%)	275 (96%)	12 (4%)	26	49
1	B	280/325 (86%)	270 (96%)	10 (4%)	31	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	567/650 (87%)	545 (96%)	22 (4%)	28 51

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	57	GLU
1	A	74	ARG
1	A	75	VAL
1	A	99	GLU
1	A	183	LYS
1	A	187	ARG
1	A	194	LYS
1	A	241	LEU
1	A	248	GLN
1	A	292	GLU
1	A	334	ARG
1	B	16	VAL
1	B	53	LYS
1	B	55	VAL
1	B	75	VAL
1	B	99	GLU
1	B	158	SER
1	B	163	GLU
1	B	182	LYS
1	B	190	GLU
1	B	268	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	195	ASN
1	A	235	HIS
1	A	246	GLN
1	A	261	ASN
1	A	264	HIS
1	A	301	ASN
1	A	327	ASN
1	B	90	GLN
1	B	246	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

### 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	324/373 (86%)	0.63	20 (6%) 26 26	37, 57, 80, 100	0
1	B	319/373 (85%)	0.58	22 (6%) 23 22	33, 52, 75, 89	0
All	All	643/746 (86%)	0.60	42 (6%) 25 24	33, 54, 77, 100	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	CYS	4.5
1	B	268	VAL	3.8
1	B	139	SER	3.8
1	A	275	ASN	3.5
1	A	58	THR	3.3
1	B	141	LEU	3.2
1	B	98	LEU	3.1
1	B	329	GLU	3.0
1	A	81	ASP	3.0
1	A	276	ILE	3.0
1	A	59	ASP	2.9
1	B	201	LEU	2.9
1	A	103	ASP	2.8
1	B	267	PRO	2.6
1	A	225	ASN	2.6
1	B	187	ARG	2.6
1	B	344	TYR	2.6
1	A	227	ASP	2.5
1	A	163	GLU	2.5
1	B	55	VAL	2.5
1	A	118	GLU	2.5
1	A	264	HIS	2.4
1	B	144	GLN	2.4
1	B	37	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	16	VAL	2.4
1	A	37	ALA	2.3
1	B	168	ASP	2.3
1	B	264	HIS	2.2
1	B	247	ASP	2.2
1	A	27	VAL	2.2
1	B	233	GLY	2.2
1	A	22	TYR	2.1
1	B	38	LEU	2.1
1	A	54	PHE	2.1
1	B	269	ALA	2.1
1	A	69	ASN	2.1
1	A	335	ASP	2.1
1	B	236	SER	2.1
1	A	305	SER	2.0
1	B	92	ILE	2.0
1	B	77	GLU	2.0
1	A	141	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 oligosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	B	400	1/1	0.86	0.25	40,40,40,40	0
2	NA	A	400	1/1	0.90	0.17	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.