



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:05 am BST

PDB ID : 6DX7  
Title : Crystal structure of chalcone synthase from *Physcomitrella patens*  
Authors : Liou, G.; Chiang, Y.C.; Wang, Y.; Weng, J.K.  
Deposited on : 2018-06-28  
Resolution : 2.61 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

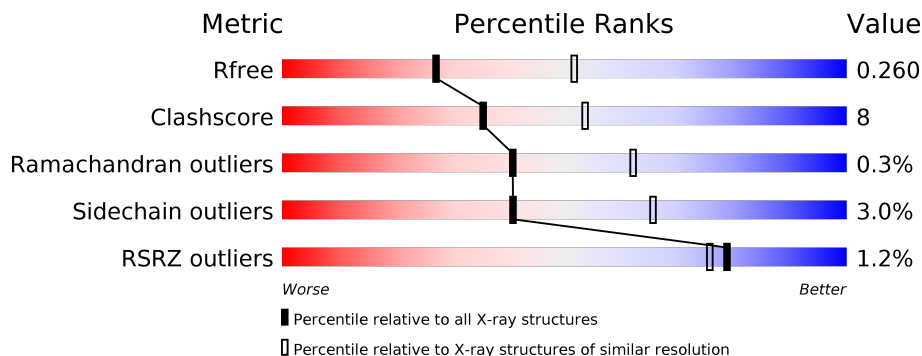
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 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	397	
1	B	397	
1	C	397	
1	D	397	
1	E	397	
1	F	397	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 35469 atoms, of which 17818 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 Chalcone synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	387	5902	1871	2970	510	536	15	0	0	0
1	B	387	5902	1871	2970	510	536	15	0	0	0
1	C	387	5902	1871	2970	510	536	15	0	0	0
1	D	387	5902	1871	2970	510	536	15	0	0	0
1	E	387	5902	1871	2970	510	536	15	0	0	0
1	F	387	5900	1871	2968	510	536	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLU	ASP	variant	UNP Q2VAZ3
B	44	GLU	ASP	variant	UNP Q2VAZ3
C	44	GLU	ASP	variant	UNP Q2VAZ3
D	44	GLU	ASP	variant	UNP Q2VAZ3
E	44	GLU	ASP	variant	UNP Q2VAZ3
F	44	GLU	ASP	variant	UNP Q2VAZ3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total 14	O 14	0	0
2	B	8	Total 8	O 8	0	0
2	C	13	Total 13	O 13	0	0

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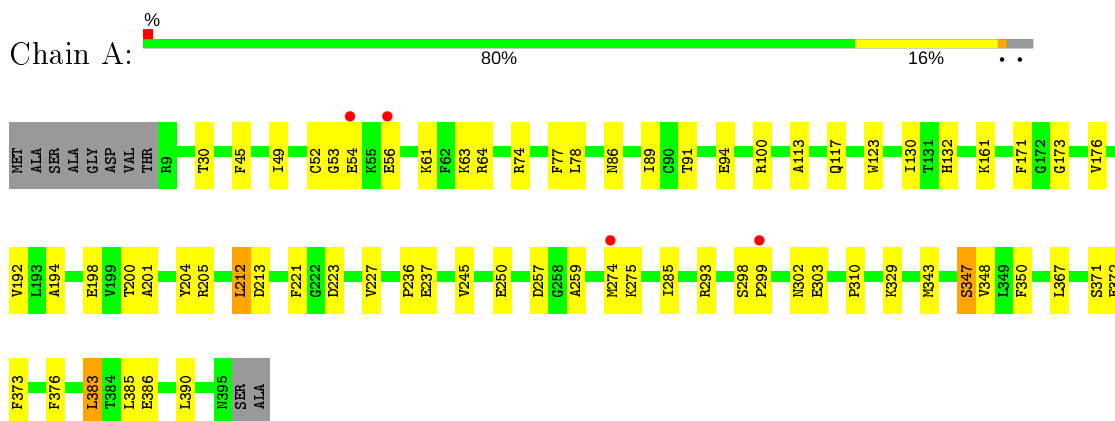
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
2	D	7	Total O 7 7	0	0
2	E	6	Total O 6 6	0	0
2	F	11	Total O 11 11	0	0

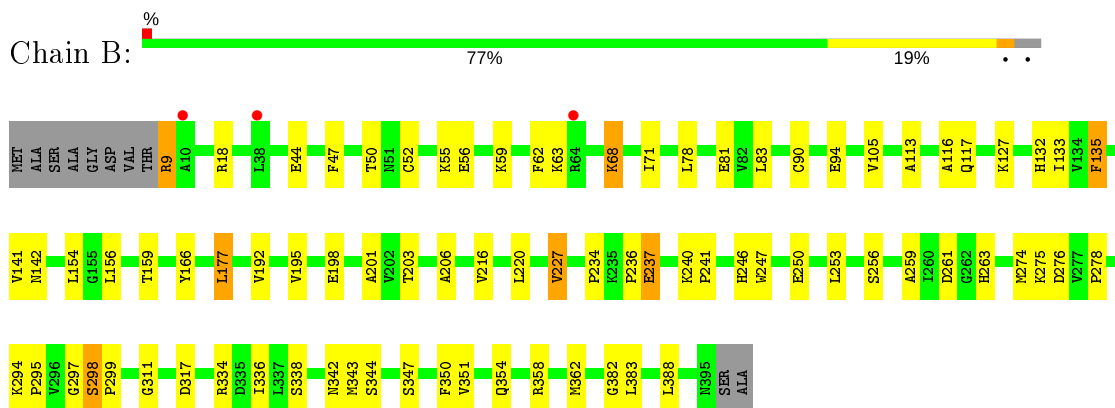
### 3 Residue-property plots [i](#)

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.

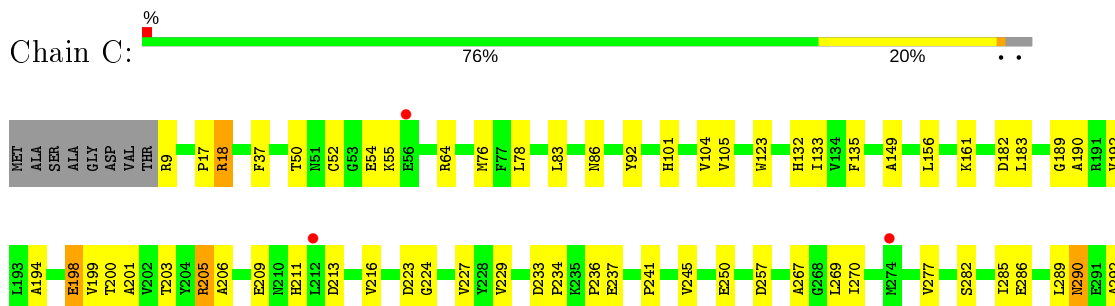
- Molecule 1: Chalcone synthase



- Molecule 1: Chalcone synthase

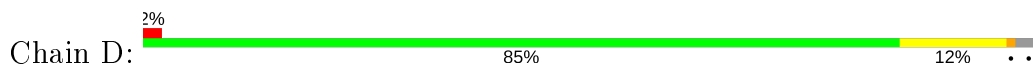


- Molecule 1: Chalcone synthase

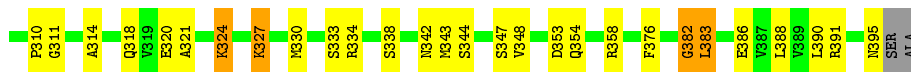
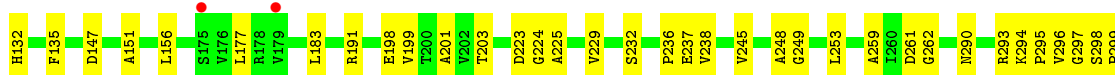
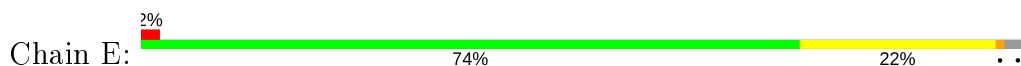




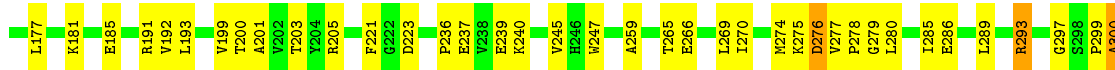
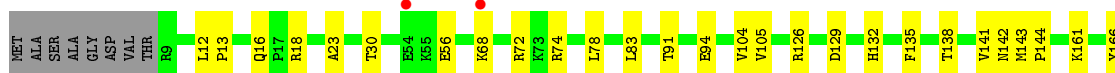
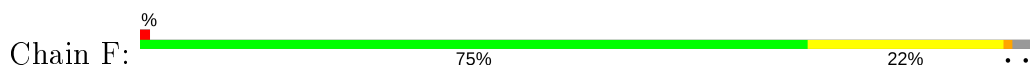
- Molecule 1: Chalcone synthase



- Molecule 1: Chalcone synthase



- Molecule 1: Chalcone synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.60Å 192.83Å 195.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.01 – 2.61 37.01 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.01-2.61) 99.0 (37.01-2.61)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.181 , 0.263 0.180 , 0.260	Depositor DCC
$R_{free}$ test set	1967 reflections (2.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtrriage
Anisotropy	0.717	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	35469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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

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	0.71	0/2996	0.76	0/4053
1	B	0.67	1/2996 (0.0%)	0.74	0/4053
1	C	0.68	1/2996 (0.0%)	0.74	2/4053 (0.0%)
1	D	0.64	1/2996 (0.0%)	0.72	1/4053 (0.0%)
1	E	0.60	0/2996	0.72	1/4053 (0.0%)
1	F	0.66	0/2996	0.72	1/4053 (0.0%)
All	All	0.66	3/17976 (0.0%)	0.73	5/24318 (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	B	0	1
1	E	0	1
1	F	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	GLU	CG-CD	7.26	1.62	1.51
1	B	227	VAL	CB-CG1	-5.23	1.41	1.52
1	D	18	ARG	NE-CZ	5.21	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	18	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	233	ASP	CB-CG-OD1	6.29	123.96	118.30
1	E	14	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	F	390	LEU	CB-CG-CD2	5.60	120.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	ASP	CB-CG-OD1	5.26	123.04	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	382	GLY	Peptide
1	E	382	GLY	Peptide
1	F	382	GLY	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	2932	2970	2970	44	0
1	B	2932	2970	2970	48	0
1	C	2932	2970	2970	55	1
1	D	2932	2970	2970	27	1
1	E	2932	2970	2970	58	0
1	F	2932	2968	2970	69	0
2	A	14	0	0	2	0
2	B	8	0	0	0	0
2	C	13	0	0	5	0
2	D	7	0	0	0	0
2	E	6	0	0	0	0
2	F	11	0	0	0	0
All	All	17651	17818	17820	288	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 8.

All (288) 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:F:293:ARG:NE	1:F:299:PRO:O	1.93	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:NH2	1:C:267:ALA:O	2.05	0.90
1:A:77:PHE:O	2:A:401:HOH:O	1.91	0.86
1:A:212:LEU:HD12	1:A:213:ASP:H	1.45	0.81
1:A:293:ARG:HB3	1:A:298:SER:HA	1.64	0.80
1:C:277:VAL:HG13	1:C:383:LEU:HD11	1.64	0.79
1:F:299:PRO:HB3	1:F:300:ALA:HB3	1.66	0.77
1:C:395:ASN:OD1	2:C:402:HOH:O	2.05	0.74
1:A:200:THR:HG23	1:A:223:ASP:OD1	1.89	0.73
1:A:205:ARG:HB3	1:A:205:ARG:CZ	2.19	0.71
1:D:293:ARG:HB3	1:D:298:SER:HA	1.74	0.70
1:C:9:ARG:NE	2:C:401:HOH:O	1.97	0.70
1:C:245:VAL:HG12	1:C:390:LEU:HD22	1.76	0.68
1:C:213:ASP:O	1:C:216:VAL:HG12	1.93	0.68
1:F:205:ARG:CZ	1:F:205:ARG:HB3	2.23	0.68
1:F:72:ARG:NH1	1:F:339:GLU:OE2	2.28	0.67
1:A:45:PHE:O	1:A:49:ILE:HD12	1.95	0.67
1:B:253:LEU:HD12	1:B:383:LEU:HD12	1.77	0.66
1:A:257:ASP:OD2	2:A:402:HOH:O	2.14	0.66
1:B:216:VAL:O	1:B:220:LEU:HD12	1.95	0.65
1:C:50:THR:HG21	1:C:206:ALA:HA	1.79	0.65
1:E:111:LEU:HD22	1:E:225:ALA:HB3	1.80	0.64
1:E:113:ALA:O	1:E:117:GLN:HG2	1.98	0.64
1:E:311:GLY:HA2	1:E:342:ASN:HD22	1.62	0.62
1:F:293:ARG:NH2	1:F:300:ALA:H	1.96	0.62
1:F:104:VAL:HG12	1:F:199:VAL:HG22	1.81	0.62
1:C:92:TYR:O	1:C:205:ARG:NH1	2.31	0.62
1:B:259:ALA:HB3	1:B:383:LEU:HD23	1.82	0.62
1:E:320:GLU:OE1	1:E:334:ARG:NH2	2.30	0.62
1:E:253:LEU:HD12	1:E:383:LEU:HD12	1.83	0.60
1:E:297:GLY:O	1:E:299:PRO:HD3	2.01	0.60
1:C:367:LEU:HD22	1:C:393:ALA:HB3	1.83	0.60
1:E:73:LYS:NZ	1:E:75:HIS:NE2	2.49	0.59
1:F:299:PRO:CB	1:F:300:ALA:HB3	2.31	0.59
1:D:198:GLU:HG3	1:D:343:MET:O	2.01	0.59
1:B:259:ALA:HA	1:B:275:LYS:HG3	1.83	0.59
1:C:203:THR:HG22	1:C:269:LEU:HD23	1.84	0.58
1:A:30:THR:HB	1:A:350:PHE:CZ	2.38	0.58
1:C:101:HIS:O	1:C:105:VAL:HG12	2.03	0.58
1:B:236:PRO:O	1:B:237:GLU:HB2	2.03	0.58
1:E:71:ILE:HA	1:E:338:SER:HA	1.86	0.58
1:E:11:ALA:HA	1:F:391:ARG:HH12	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:HIS:HB2	1:B:192:VAL:HG22	1.86	0.57
1:A:161:LYS:HA	1:B:250:GLU:OE2	2.03	0.57
1:F:203:THR:HG22	1:F:269:LEU:HD23	1.86	0.57
1:B:336:ILE:HD12	1:B:350:PHE:HB3	1.86	0.57
1:E:321:ALA:O	1:E:324:LYS:HE3	2.04	0.57
1:A:132:HIS:HB2	1:A:192:VAL:HG22	1.86	0.57
1:C:236:PRO:O	1:C:237:GLU:HB2	2.06	0.56
1:D:73:LYS:NZ	1:D:75:HIS:NE2	2.54	0.56
1:F:236:PRO:O	1:F:237:GLU:HB2	2.05	0.55
1:E:290:ASN:HA	1:E:293:ARG:HD2	1.88	0.55
1:C:234:PRO:HG2	1:C:241:PRO:HG3	1.88	0.55
1:E:236:PRO:O	1:E:237:GLU:HB2	2.07	0.55
1:E:78:LEU:HD11	1:E:201:ALA:HA	1.89	0.54
1:C:92:TYR:HA	1:C:206:ALA:HB3	1.89	0.54
1:E:27:GLY:HA2	1:E:122:GLU:HG2	1.89	0.54
1:F:293:ARG:CZ	1:F:299:PRO:O	2.55	0.54
1:F:278:PRO:HG3	1:F:315:ILE:HG13	1.89	0.54
1:C:205:ARG:CB	1:C:205:ARG:CZ	2.86	0.54
1:F:299:PRO:HA	1:F:300:ALA:CB	2.38	0.53
1:C:37:PHE:CE1	1:C:76:MET:HB2	2.43	0.53
1:E:249:GLY:HA2	1:F:161:LYS:HE3	1.89	0.53
1:E:293:ARG:NH2	1:E:299:PRO:O	2.41	0.53
1:C:200:THR:HG23	1:C:223:ASP:OD1	2.09	0.53
1:E:238:VAL:HG22	1:E:238:VAL:O	2.08	0.53
1:C:372:GLU:HG2	1:C:373:PHE:CD2	2.44	0.53
1:A:250:GLU:HB3	1:A:386:GLU:HG2	1.91	0.52
1:D:132:HIS:HA	1:D:161:LYS:O	2.09	0.52
1:B:216:VAL:HG12	1:B:220:LEU:HD13	1.91	0.52
1:F:293:ARG:CD	1:F:299:PRO:O	2.56	0.52
1:C:293:ARG:HB3	1:C:298:SER:HA	1.92	0.52
1:F:200:THR:HG23	1:F:223:ASP:OD1	2.08	0.52
1:A:52:CYS:O	1:A:54:GLU:N	2.41	0.52
1:D:78:LEU:HD11	1:D:201:ALA:HA	1.91	0.52
1:F:126:ARG:NH1	1:F:129:ASP:OD2	2.43	0.52
1:C:205:ARG:HB3	1:C:205:ARG:CZ	2.39	0.52
1:A:45:PHE:CD1	1:A:49:ILE:HD13	2.45	0.51
1:A:52:CYS:C	1:A:54:GLU:H	2.12	0.51
1:B:47:PHE:CZ	1:B:59:LYS:HA	2.45	0.51
1:F:259:ALA:HA	1:F:274:MET:HB2	1.92	0.51
1:B:133:ILE:HD11	1:B:156:LEU:HD12	1.92	0.51
1:E:311:GLY:HA2	1:E:342:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PRO:O	1:A:237:GLU:HB2	2.11	0.51
1:C:205:ARG:HB2	1:C:205:ARG:NH1	2.25	0.51
1:E:354:GLN:O	1:E:358:ARG:HG3	2.11	0.51
1:F:276:ASP:O	1:F:280:LEU:HG	2.10	0.51
1:D:320:GLU:OE2	1:D:334:ARG:NH2	2.44	0.51
1:C:315:ILE:HG21	1:C:379:PHE:CZ	2.46	0.51
1:D:38:LEU:HD23	1:D:72:ARG:O	2.11	0.51
1:F:265:THR:HG21	1:F:270:ILE:HD13	1.93	0.51
1:F:315:ILE:HG21	1:F:379:PHE:CZ	2.44	0.51
1:D:132:HIS:HB2	1:D:192:VAL:HG22	1.92	0.51
1:F:299:PRO:CA	1:F:300:ALA:HB3	2.41	0.51
1:E:199:VAL:HG23	1:E:223:ASP:OD2	2.10	0.51
1:E:310:PRO:HD2	1:E:347:SER:HB3	1.92	0.50
1:F:91:THR:OG1	1:F:94:GLU:HB2	2.11	0.50
1:F:68:LYS:O	1:F:313:PRO:HG3	2.12	0.50
1:A:212:LEU:HD13	1:A:213:ASP:CG	2.31	0.50
1:B:78:LEU:HD11	1:B:201:ALA:HA	1.91	0.50
1:C:203:THR:CG2	1:C:269:LEU:HD23	2.42	0.50
1:F:30:THR:HB	1:F:350:PHE:CZ	2.46	0.50
1:E:294:LYS:HB2	1:E:295:PRO:HD3	1.93	0.50
1:C:194:ALA:O	1:C:227:VAL:HA	2.11	0.50
1:C:211:HIS:CE1	1:C:270:ILE:HG23	2.47	0.50
1:C:290:ASN:OD1	1:C:293:ARG:NH2	2.44	0.50
1:D:349:LEU:CD2	1:D:376:PHE:HZ	2.25	0.50
1:A:45:PHE:O	1:A:49:ILE:CD1	2.59	0.49
1:E:259:ALA:HB3	1:E:383:LEU:HD23	1.93	0.49
1:F:259:ALA:HB3	1:F:383:LEU:HD23	1.94	0.49
1:B:336:ILE:HG13	1:B:351:VAL:HA	1.94	0.49
1:A:194:ALA:O	1:A:227:VAL:HA	2.12	0.49
1:E:132:HIS:CD2	1:E:183:LEU:HD23	2.48	0.49
1:A:78:LEU:HD11	1:A:201:ALA:HA	1.95	0.49
1:D:127:LYS:HD2	1:D:154:LEU:O	2.12	0.49
1:E:327:LYS:HD2	1:E:327:LYS:N	2.27	0.49
1:E:52:CYS:SG	1:E:55:LYS:HE3	2.52	0.49
1:F:285:ILE:HG23	1:F:286:GLU:N	2.27	0.49
1:F:105:VAL:HG22	1:F:142:ASN:HB2	1.95	0.49
1:F:299:PRO:CA	1:F:300:ALA:CB	2.91	0.49
1:A:259:ALA:HB3	1:A:383:LEU:HD23	1.94	0.49
1:C:331:GLN:HG2	1:C:358:ARG:NH2	2.27	0.48
1:E:382:GLY:H	1:F:144:PRO:HG3	1.78	0.48
1:F:74:ARG:NH1	1:F:221:PHE:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:PRO:HD2	1:F:347:SER:HB3	1.94	0.48
1:D:349:LEU:HD23	1:D:376:PHE:HZ	1.78	0.48
1:E:314:ALA:O	1:E:318:GLN:HG3	2.14	0.48
1:E:111:LEU:HD22	1:E:225:ALA:CB	2.42	0.48
1:D:89:ILE:O	1:D:89:ILE:HG22	2.13	0.48
1:E:37:PHE:CE1	1:E:76:MET:HB2	2.48	0.48
1:C:344:SER:OG	1:C:345:SER:N	2.46	0.48
1:E:293:ARG:HG3	1:E:298:SER:HA	1.95	0.48
1:E:348:VAL:HG13	1:E:376:PHE:CZ	2.49	0.48
1:A:198:GLU:HG3	1:A:343:MET:O	2.14	0.47
1:F:12:LEU:HD13	1:F:13:PRO:HD2	1.96	0.47
1:A:212:LEU:CD1	1:A:213:ASP:H	2.23	0.47
1:E:248:ALA:HB2	1:E:388:LEU:HD23	1.97	0.47
1:B:81:GLU:CD	1:B:81:GLU:H	2.18	0.47
1:F:304:MET:HA	1:F:373:PHE:O	2.13	0.47
1:D:236:PRO:O	1:D:237:GLU:HB2	2.14	0.47
1:E:98:ASN:OD1	1:F:266:GLU:HG3	2.14	0.47
1:E:330:MET:CE	1:E:333:SER:HB2	2.45	0.47
1:E:33:PRO:HD3	1:E:111:LEU:HD11	1.97	0.47
1:D:302:ASN:O	1:D:329:LYS:NZ	2.30	0.46
1:F:276:ASP:OD1	1:F:279:GLY:N	2.41	0.46
1:A:274:MET:O	1:A:275:LYS:HG3	2.15	0.46
1:B:127:LYS:HD2	1:B:154:LEU:O	2.16	0.46
1:D:281:ILE:HG21	1:D:315:ILE:HD11	1.97	0.46
1:E:100:ARG:NH1	1:E:201:ALA:O	2.49	0.46
1:E:391:ARG:NH1	1:F:12:LEU:HD23	2.31	0.46
1:C:78:LEU:HD11	1:C:201:ALA:HA	1.98	0.46
1:A:86:ASN:HB3	1:A:89:ILE:HD12	1.98	0.46
1:B:113:ALA:O	1:B:117:GLN:HG2	2.15	0.46
1:C:285:ILE:HG23	1:C:286:GLU:N	2.31	0.46
1:C:9:ARG:NH2	2:C:401:HOH:O	2.48	0.46
1:E:262:GLY:HA3	1:F:143:MET:HB2	1.97	0.46
1:B:294:LYS:HB2	1:B:295:PRO:HD3	1.98	0.45
1:C:250:GLU:HB3	1:C:386:GLU:HG2	1.97	0.45
1:E:28:ILE:HG21	1:E:353:ASP:HB2	1.97	0.45
1:F:285:ILE:HG12	1:F:289:LEU:HD11	1.97	0.45
1:C:149:ALA:O	2:C:403:HOH:O	2.21	0.45
1:F:141:VAL:HA	1:F:166:TYR:CE1	2.52	0.45
1:A:212:LEU:HD12	1:A:213:ASP:N	2.21	0.45
1:A:372:GLU:HG2	1:A:373:PHE:CD2	2.51	0.45
1:B:261:ASP:OD1	1:B:263:HIS:CE1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HB3	1:B:90:CYS:SG	2.57	0.45
1:C:133:ILE:HD11	1:C:156:LEU:HD12	1.98	0.45
1:C:52:CYS:C	1:C:54:GLU:H	2.19	0.45
1:A:113:ALA:O	1:A:117:GLN:HG2	2.17	0.45
1:A:205:ARG:CB	1:A:205:ARG:CZ	2.93	0.45
1:B:116:ALA:HA	1:B:227:VAL:HG11	1.98	0.45
1:E:245:VAL:HG22	1:E:390:LEU:HD22	1.97	0.45
1:C:132:HIS:HB2	1:C:192:VAL:HG22	1.99	0.45
1:C:320:GLU:HA	1:C:325:LEU:HD12	1.98	0.45
1:D:101:HIS:HA	1:D:104:VAL:HG22	1.98	0.45
1:B:276:ASP:OD1	1:B:278:PRO:HD2	2.17	0.45
1:B:50:THR:HG21	1:B:206:ALA:HA	1.99	0.45
1:C:104:VAL:HG12	1:C:199:VAL:CG2	2.47	0.45
1:C:189:GLY:O	1:C:190:ALA:C	2.54	0.45
1:C:372:GLU:HG2	1:C:373:PHE:CE2	2.51	0.45
1:B:116:ALA:CA	1:B:227:VAL:HG11	2.47	0.44
1:F:23:ALA:O	1:F:245:VAL:HG12	2.17	0.44
1:F:275:LYS:HD3	1:F:276:ASP:H	1.82	0.44
1:A:74:ARG:HD2	1:A:221:PHE:O	2.17	0.44
1:A:310:PRO:HD2	1:A:347:SER:HB2	1.99	0.44
1:C:315:ILE:HD12	1:C:315:ILE:H	1.83	0.44
1:D:259:ALA:O	1:D:273:LEU:HA	2.18	0.44
1:E:296:VAL:C	1:E:297:GLY:O	2.49	0.44
1:D:224:GLY:HA3	1:D:343:MET:SD	2.58	0.44
1:F:181:LYS:NZ	1:F:185:GLU:OE1	2.49	0.44
1:F:265:THR:CG2	1:F:270:ILE:HD13	2.47	0.44
1:E:98:ASN:CG	1:F:266:GLU:HG3	2.37	0.44
1:A:100:ARG:NH1	1:A:204:TYR:O	2.48	0.44
1:F:78:LEU:HD11	1:F:201:ALA:HA	2.00	0.44
1:B:47:PHE:HE1	1:B:62:PHE:CD2	2.36	0.44
1:F:293:ARG:NH2	1:F:301:TRP:CD2	2.86	0.44
1:A:86:ASN:CB	1:A:89:ILE:HD12	2.48	0.44
1:C:123:TRP:CG	1:C:229:VAL:HG11	2.53	0.44
1:A:171:PHE:CD1	1:A:171:PHE:C	2.91	0.43
1:A:348:VAL:HG13	1:A:376:PHE:CZ	2.53	0.43
1:F:278:PRO:HB3	1:F:315:ILE:HA	2.00	0.43
1:E:224:GLY:HA3	1:E:343:MET:SD	2.59	0.43
1:E:198:GLU:HG3	1:E:343:MET:O	2.18	0.43
1:F:247:TRP:HB3	1:F:389:VAL:HB	1.99	0.43
1:D:310:PRO:HD3	1:D:351:VAL:HG21	2.00	0.43
1:B:68:LYS:C	1:B:68:LYS:HD2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:HIS:HA	1:C:161:LYS:O	2.18	0.43
1:E:16:GLN:OE1	1:F:247:TRP:HA	2.19	0.43
1:B:343:MET:N	1:B:347:SER:OG	2.48	0.43
1:D:290:ASN:OD1	1:D:293:ARG:NH2	2.52	0.43
1:F:275:LYS:O	1:F:277:VAL:N	2.51	0.43
1:F:367:LEU:CD1	1:F:395:ASN:HB2	2.49	0.43
1:B:198:GLU:OE2	1:B:344:SER:OG	2.31	0.43
1:B:247:TRP:O	1:B:388:LEU:HA	2.19	0.43
1:E:123:TRP:CD2	1:E:229:VAL:HG11	2.54	0.43
1:C:292:ALA:O	1:C:295:PRO:HD2	2.19	0.43
1:F:132:HIS:HA	1:F:161:LYS:O	2.19	0.43
1:A:303:GLU:O	1:A:371:SER:HB3	2.19	0.42
1:A:302:ASN:HA	1:A:329:LYS:HE3	2.01	0.42
1:D:141:VAL:HG12	1:D:166:TYR:CG	2.53	0.42
1:D:177:LEU:HA	1:D:177:LEU:HD23	1.92	0.42
1:D:104:VAL:HG11	1:D:202:VAL:HG23	2.00	0.42
1:E:104:VAL:HG12	1:E:199:VAL:HG13	2.01	0.42
1:F:191:ARG:NH2	1:F:239:GLU:OE1	2.47	0.42
1:C:198:GLU:HG3	1:C:343:MET:O	2.19	0.42
1:B:274:MET:O	1:B:275:LYS:HG2	2.19	0.42
1:C:104:VAL:CG1	1:C:201:ALA:HB3	2.49	0.42
1:D:293:ARG:HD2	1:D:299:PRO:O	2.20	0.42
1:D:36:GLU:HG2	1:D:75:HIS:CE1	2.54	0.42
1:E:151:ALA:HA	1:E:156:LEU:HD12	2.00	0.42
1:C:104:VAL:HG12	1:C:199:VAL:HG23	2.01	0.42
1:A:245:VAL:HG22	1:A:390:LEU:HD22	2.02	0.42
1:B:116:ALA:N	1:B:227:VAL:HG11	2.34	0.42
1:B:317:ASP:OD1	1:B:334:ARG:NH1	2.53	0.42
1:B:358:ARG:O	1:B:362:MET:HG2	2.20	0.42
1:E:9:ARG:NH1	1:E:10:ALA:H	2.18	0.42
1:E:253:LEU:CD1	1:E:383:LEU:HD12	2.48	0.42
1:B:234:PRO:HG2	1:B:241:PRO:HG3	2.00	0.42
1:C:9:ARG:CZ	2:C:401:HOH:O	2.55	0.42
1:D:97:LEU:HA	1:D:100:ARG:HD2	2.01	0.42
1:F:132:HIS:HB2	1:F:192:VAL:HG22	2.01	0.42
1:B:71:ILE:HA	1:B:338:SER:HA	2.01	0.42
1:E:147:ASP:N	1:E:147:ASP:OD1	2.53	0.42
1:E:191:ARG:HD3	1:E:191:ARG:HA	1.81	0.42
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.92	0.41
1:B:256:SER:OG	1:B:383:LEU:HB2	2.20	0.41
1:C:78:LEU:HB3	1:C:83:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:ALA:H	1:F:16:GLN:HE22	1.68	0.41
1:B:297:GLY:O	1:B:299:PRO:HD3	2.20	0.41
1:F:104:VAL:HG13	1:F:201:ALA:HB3	2.02	0.41
1:B:105:VAL:HG22	1:B:142:ASN:HB2	2.02	0.41
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.82	0.41
1:F:83:LEU:HD23	1:F:83:LEU:HA	1.95	0.41
1:F:383:LEU:HD13	1:F:383:LEU:HA	1.82	0.41
1:A:91:THR:OG1	1:A:94:GLU:HG2	2.21	0.41
1:C:132:HIS:CD2	1:C:183:LEU:HD23	2.56	0.41
1:E:31:ALA:O	1:E:111:LEU:HD21	2.21	0.41
1:F:354:GLN:O	1:F:358:ARG:HG3	2.21	0.41
1:B:274:MET:HG3	1:F:339:GLU:HG3	2.03	0.41
1:F:380:GLY:O	1:F:383:LEU:HA	2.21	0.41
1:C:203:THR:HG22	1:C:269:LEU:HB3	2.03	0.41
1:C:55:LYS:NZ	1:C:209:GLU:OE1	2.52	0.41
1:C:224:GLY:HA3	1:C:343:MET:SD	2.60	0.41
1:B:311:GLY:HA2	1:B:342:ASN:ND2	2.35	0.41
1:E:42:TYR:N	1:E:43:PRO:CD	2.84	0.41
1:A:123:TRP:CZ3	1:A:130:ILE:HD11	2.56	0.41
1:B:336:ILE:HD11	1:B:354:GLN:HB2	2.02	0.41
1:F:285:ILE:HG12	1:F:289:LEU:CD1	2.51	0.41
1:A:298:SER:N	1:A:299:PRO:CD	2.83	0.41
1:B:135:PHE:HA	1:B:195:VAL:O	2.21	0.41
1:B:9:ARG:HA	1:B:9:ARG:HD3	1.89	0.41
1:B:44:GLU:OE1	1:B:44:GLU:N	2.53	0.40
1:D:24:CYS:O	1:D:230:VAL:HA	2.21	0.40
1:F:297:GLY:C	1:F:299:PRO:HD3	2.41	0.40
1:F:320:GLU:OE2	1:F:330:MET:HB2	2.21	0.40
1:C:347:SER:O	1:C:351:VAL:HG23	2.22	0.40
1:E:92:TYR:O	1:E:93:MET:HG2	2.21	0.40
1:F:337:LEU:HD12	1:F:341:GLY:HA2	2.02	0.40
1:A:173:GLY:O	1:A:176:VAL:HG22	2.20	0.40
1:A:212:LEU:CD1	1:A:213:ASP:N	2.84	0.40
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.89	0.40
1:F:193:LEU:HD23	1:F:193:LEU:HA	1.87	0.40
1:A:250:GLU:O	1:B:159:THR:HA	2.21	0.40
1:B:52:CYS:SG	1:B:55:LYS:NZ	2.81	0.40
1:A:285:ILE:HD12	1:A:385:LEU:HD21	2.04	0.40
1:B:141:VAL:HG12	1:B:166:TYR:CG	2.56	0.40
1:B:240:LYS:O	1:B:240:LYS:HG3	2.22	0.40
1:E:391:ARG:HH12	1:F:12:LEU:HD23	1.85	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:C:18:ARG:HH21	1:D:18:ARG:HE[1_455]	1.31	0.29

## 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	385/397 (97%)	362 (94%)	22 (6%)	1 (0%)	41 62
1	B	385/397 (97%)	363 (94%)	21 (6%)	1 (0%)	41 62
1	C	385/397 (97%)	363 (94%)	21 (6%)	1 (0%)	41 62
1	D	385/397 (97%)	364 (94%)	20 (5%)	1 (0%)	41 62
1	E	385/397 (97%)	360 (94%)	24 (6%)	1 (0%)	41 62
1	F	385/397 (97%)	361 (94%)	21 (6%)	3 (1%)	19 36
All	All	2310/2382 (97%)	2173 (94%)	129 (6%)	8 (0%)	41 62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	276	ASP
1	F	300	ALA
1	F	383	LEU
1	C	17	PRO
1	E	14	ARG
1	A	53	GLY
1	D	296	VAL
1	B	298	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/314 (98%)	300 (97%)	8 (3%)	46	70
1	B	308/314 (98%)	296 (96%)	12 (4%)	32	56
1	C	308/314 (98%)	300 (97%)	8 (3%)	46	70
1	D	308/314 (98%)	302 (98%)	6 (2%)	57	78
1	E	308/314 (98%)	296 (96%)	12 (4%)	32	56
1	F	308/314 (98%)	299 (97%)	9 (3%)	42	67
All	All	1848/1884 (98%)	1793 (97%)	55 (3%)	41	66

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	61	LYS
1	A	63	LYS
1	A	64	ARG
1	A	212	LEU
1	A	347	SER
1	A	367	LEU
1	A	383	LEU
1	B	9	ARG
1	B	18	ARG
1	B	56	GLU
1	B	63	LYS
1	B	68	LYS
1	B	94	GLU
1	B	135	PHE
1	B	177	LEU
1	B	203	THR
1	B	237	GLU
1	B	246	HIS
1	B	298	SER
1	C	18	ARG
1	C	64	ARG

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Mol	Chain	Res	Type
1	C	86	ASN
1	C	135	PHE
1	C	205	ARG
1	C	257	ASP
1	C	282	SER
1	C	290	ASN
1	D	94	GLU
1	D	135	PHE
1	D	138	THR
1	D	177	LEU
1	D	218	SER
1	D	244	GLU
1	E	12	LEU
1	E	135	PHE
1	E	177	LEU
1	E	203	THR
1	E	232	SER
1	E	261	ASP
1	E	324	LYS
1	E	327	LYS
1	E	344	SER
1	E	383	LEU
1	E	386	GLU
1	E	395	ASN
1	F	18	ARG
1	F	56	GLU
1	F	135	PHE
1	F	138	THR
1	F	240	LYS
1	F	293	ARG
1	F	324	LYS
1	F	330	MET
1	F	349	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

#### 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	387/397 (97%)	-0.26	4 (1%) 82 80	28, 50, 104, 139	0
1	B	387/397 (97%)	-0.26	3 (0%) 86 84	32, 55, 90, 161	0
1	C	387/397 (97%)	-0.20	3 (0%) 86 84	32, 56, 110, 179	0
1	D	387/397 (97%)	-0.18	9 (2%) 60 55	36, 59, 92, 130	0
1	E	387/397 (97%)	-0.18	7 (1%) 68 64	40, 66, 102, 206	0
1	F	387/397 (97%)	0.01	3 (0%) 86 84	32, 62, 108, 130	0
All	All	2322/2382 (97%)	-0.18	29 (1%) 79 76	28, 58, 103, 206	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	11	ALA	9.6
1	E	9	ARG	4.8
1	E	10	ALA	4.3
1	E	12	LEU	4.1
1	E	13	PRO	4.1
1	C	56	GLU	3.2
1	F	68	LYS	3.2
1	A	299	PRO	3.1
1	D	134	VAL	3.0
1	A	274	MET	3.0
1	D	176	VAL	2.9
1	B	64	ARG	2.8
1	D	173	GLY	2.7
1	A	56	GLU	2.6
1	D	194	ALA	2.6
1	F	54	GLU	2.5
1	E	175	SER	2.4
1	C	212	LEU	2.4
1	C	274	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	54	GLU	2.3
1	D	163	VAL	2.3
1	D	136	ALA	2.3
1	B	38	LEU	2.3
1	D	237	GLU	2.2
1	E	179	VAL	2.2
1	B	10	ALA	2.1
1	D	135	PHE	2.0
1	D	177	LEU	2.0
1	F	351	VAL	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.