



# Full wwPDB X-ray Structure Validation Report i

Aug 15, 2023 – 12:09 PM JST

PDB ID : 8H6Q  
Title : Class I sesquiterpene synthase BCBOT2 (apo)  
Authors : Lou, T.T.; Ma, M.  
Deposited on : 2022-10-18  
Resolution : 2.00 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 i 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

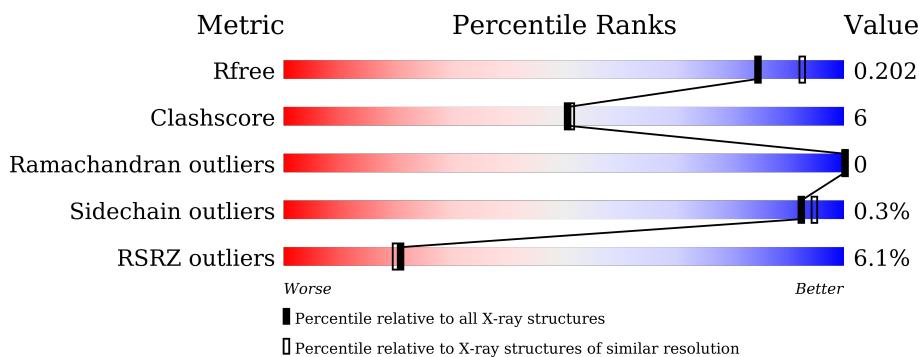
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

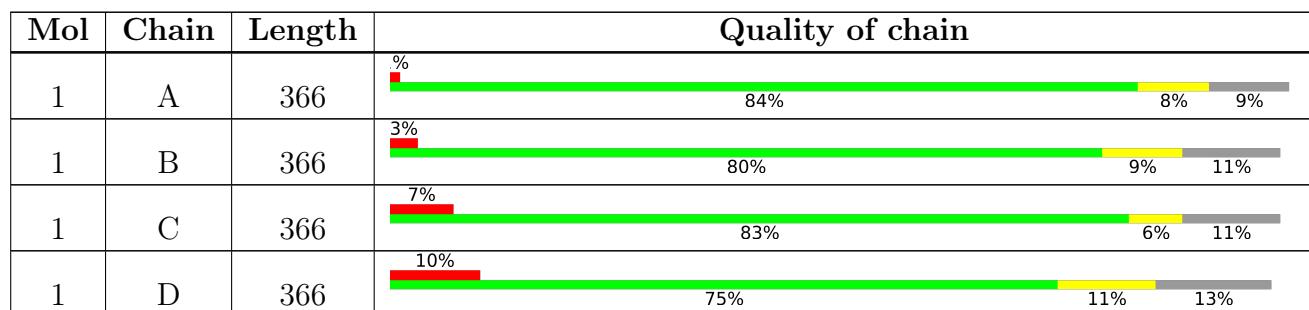
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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.



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12017 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 Presilphiperfolan-8-beta-ol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C 2691	N 1710	O 465	S 497	19	0	0
1	B	325	Total	C 2620	N 1665	O 452	S 484	19	0	0
1	C	326	Total	C 2627	N 1670	O 453	S 485	19	0	0
1	D	318	Total	C 2556	N 1619	O 445	S 473	19	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q6WP50
A	-4	SER	-	expression tag	UNP Q6WP50
A	-3	HIS	-	expression tag	UNP Q6WP50
A	-2	MET	-	expression tag	UNP Q6WP50
A	-1	ALA	-	expression tag	UNP Q6WP50
A	0	MET	-	expression tag	UNP Q6WP50
B	-5	GLY	-	expression tag	UNP Q6WP50
B	-4	SER	-	expression tag	UNP Q6WP50
B	-3	HIS	-	expression tag	UNP Q6WP50
B	-2	MET	-	expression tag	UNP Q6WP50
B	-1	ALA	-	expression tag	UNP Q6WP50
B	0	MET	-	expression tag	UNP Q6WP50
C	-5	GLY	-	expression tag	UNP Q6WP50
C	-4	SER	-	expression tag	UNP Q6WP50
C	-3	HIS	-	expression tag	UNP Q6WP50
C	-2	MET	-	expression tag	UNP Q6WP50
C	-1	ALA	-	expression tag	UNP Q6WP50
C	0	MET	-	expression tag	UNP Q6WP50
D	-5	GLY	-	expression tag	UNP Q6WP50
D	-4	SER	-	expression tag	UNP Q6WP50
D	-3	HIS	-	expression tag	UNP Q6WP50

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP Q6WP50
D	-1	ALA	-	expression tag	UNP Q6WP50
D	0	MET	-	expression tag	UNP Q6WP50

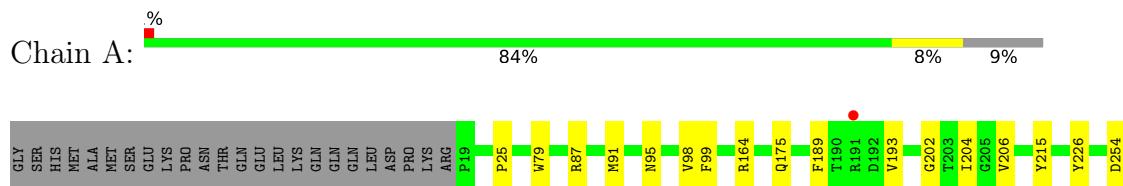
- Molecule 2 is water.

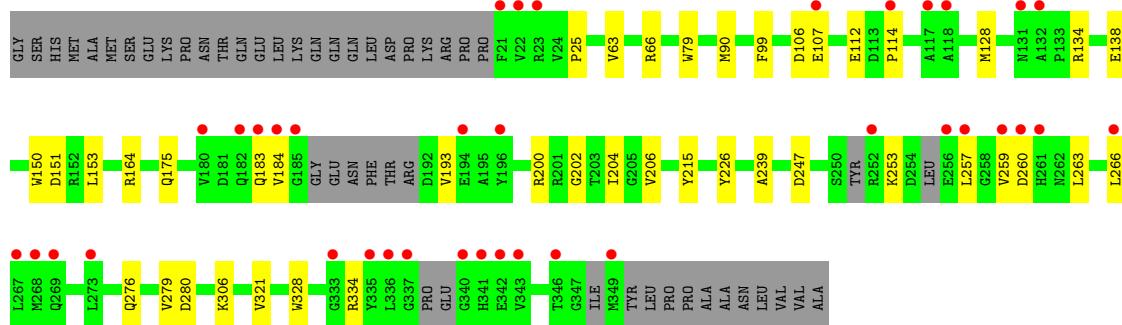
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	440	Total O 440 440	0	0
2	B	436	Total O 436 436	0	0
2	C	363	Total O 363 363	0	0
2	D	284	Total O 284 284	0	0

### 3 Residue-property plots

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: Presilphiperfolan-8-beta-ol synthase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.61Å    116.61Å    88.11Å 90.00°    111.16°    90.00°	Depositor
Resolution (Å)	40.70 – 2.00 40.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.70-2.00) 99.0 (40.70-2.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.40 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
$R$ , $R_{free}$	0.168 , 0.195 0.178 , 0.202	Depositor DCC
$R_{free}$ test set	5326 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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	0.37	0/2759	0.54	0/3746
1	B	0.40	0/2682	0.55	0/3636
1	C	0.38	0/2691	0.55	0/3651
1	D	0.35	0/2612	0.53	0/3535
All	All	0.38	0/10744	0.54	0/14568

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2691	0	2599	25	0
1	B	2620	0	2532	27	0
1	C	2627	0	2540	27	0
1	D	2556	0	2464	38	0
2	A	440	0	0	0	0
2	B	436	0	0	0	0
2	C	363	0	0	0	0
2	D	284	0	0	0	0
All	All	12017	0	10135	117	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 6.

All (117) 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:D:112:GLU:HG2	1:D:183:GLN:CG	2.00	0.91
1:A:276:GLN:O	1:A:279:VAL:HG12	1.71	0.91
1:B:204:ILE:HG23	1:B:206:VAL:HG23	1.56	0.88
1:A:175:GLN:HG3	1:A:202:GLY:HA3	1.59	0.84
1:D:112:GLU:HG2	1:D:183:GLN:HG3	1.60	0.83
1:D:175:GLN:HG3	1:D:202:GLY:HA3	1.62	0.81
1:D:276:GLN:O	1:D:279:VAL:HG12	1.82	0.80
1:D:114:PRO:HD3	1:D:184:VAL:HG21	1.64	0.78
1:D:200:ARG:O	1:D:204:ILE:HG12	1.85	0.77
1:D:112:GLU:HG2	1:D:183:GLN:HG2	1.65	0.77
1:C:254:ASP:HB3	1:C:259:VAL:HG12	1.68	0.75
1:A:25:PRO:HD3	1:A:279:VAL:HG22	1.71	0.73
1:D:193:VAL:HG22	1:D:266:LEU:HD22	1.71	0.72
1:B:276:GLN:O	1:B:279:VAL:HG12	1.90	0.72
1:D:90:MET:HE3	1:D:215:TYR:CE2	2.25	0.71
1:C:95:ASN:O	1:C:98:VAL:HG12	1.92	0.70
1:C:254:ASP:HB3	1:C:259:VAL:CG1	2.21	0.70
1:A:95:ASN:O	1:A:98:VAL:HG12	1.93	0.68
1:A:204:ILE:HG23	1:A:206:VAL:H	1.60	0.67
1:B:204:ILE:CG2	1:B:206:VAL:HG23	2.24	0.66
1:A:254:ASP:CG	1:A:259:VAL:HG11	2.17	0.66
1:B:341:HIS:O	1:B:345:GLU:HG3	1.97	0.65
1:D:138:GLU:OE1	1:D:138:GLU:N	2.30	0.65
1:D:25:PRO:HD3	1:D:279:VAL:HG22	1.79	0.64
1:D:206:VAL:HG21	1:D:239:ALA:HA	1.79	0.63
1:B:87:ARG:O	1:B:91:MET:HG3	1.98	0.63
1:A:204:ILE:HG23	1:A:206:VAL:HG23	1.82	0.61
1:A:87:ARG:O	1:A:91:MET:HG3	2.00	0.61
1:C:98:VAL:HG13	1:C:99:PHE:N	2.15	0.61
1:D:153:LEU:C	1:D:153:LEU:HD13	2.20	0.61
1:D:106:ASP:C	1:D:107:GLU:HG2	2.22	0.61
1:B:198:ASP:OD1	1:B:201:ARG:NH2	2.34	0.60
1:B:201:ARG:HG3	1:B:201:ARG:HH11	1.65	0.60
1:A:189:PHE:HB2	1:A:261:HIS:CD2	2.37	0.59
1:C:259:VAL:HG22	1:C:260:ASP:N	2.18	0.59
1:B:206:VAL:HG21	1:B:239:ALA:HA	1.84	0.59
1:B:153:LEU:C	1:B:153:LEU:HD13	2.23	0.59
1:A:204:ILE:CG2	1:A:206:VAL:HG23	2.33	0.59
1:D:114:PRO:CD	1:D:184:VAL:HG21	2.33	0.58
1:C:259:VAL:HG22	1:C:260:ASP:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ARG:HG3	1:C:201:ARG:NH1	2.18	0.57
1:A:98:VAL:HG13	1:A:99:PHE:N	2.20	0.57
1:D:90:MET:CE	1:D:215:TYR:CE2	2.89	0.56
1:C:201:ARG:HG3	1:C:201:ARG:HH11	1.71	0.56
1:B:25:PRO:HD3	1:B:279:VAL:HG22	1.87	0.55
1:B:201:ARG:HG3	1:B:201:ARG:NH1	2.19	0.55
1:B:201:ARG:HD2	1:B:207:TYR:OH	2.06	0.54
1:D:106:ASP:O	1:D:107:GLU:HG2	2.08	0.53
1:A:254:ASP:OD1	1:A:259:VAL:HG11	2.09	0.53
1:D:247:ASP:OD2	1:D:263:LEU:HB2	2.09	0.53
1:C:254:ASP:CB	1:C:259:VAL:HG12	2.39	0.52
1:D:204:ILE:HD12	1:D:206:VAL:HG23	1.91	0.52
1:C:341:HIS:O	1:C:345:GLU:HG3	2.10	0.51
1:A:254:ASP:CB	1:A:259:VAL:CG1	2.88	0.51
1:D:128:MET:HG2	1:D:150:TRP:CE3	2.46	0.51
1:D:63:VAL:HG22	1:D:66:ARG:HH12	1.76	0.51
1:B:201:ARG:HD3	1:B:236:LYS:HG3	1.92	0.50
1:D:79:TRP:CD1	1:D:321:VAL:HA	2.46	0.50
1:B:60:ASN:OD1	1:B:63:VAL:N	2.24	0.50
1:B:236:LYS:HG2	1:B:292:ARG:HH22	1.77	0.50
1:A:254:ASP:CG	1:A:259:VAL:CG1	2.80	0.50
1:B:236:LYS:HG2	1:B:292:ARG:NH2	2.27	0.50
1:D:193:VAL:HG22	1:D:266:LEU:CD2	2.41	0.49
1:C:198:ASP:OD1	1:C:201:ARG:NH2	2.45	0.49
1:A:98:VAL:CG1	1:A:99:PHE:N	2.76	0.49
1:C:95:ASN:HA	1:C:98:VAL:HG12	1.95	0.49
1:C:349:MET:HG2	1:C:349:MET:O	2.13	0.49
1:C:99:PHE:C	1:C:99:PHE:CD1	2.86	0.48
1:C:95:ASN:O	1:C:98:VAL:CG1	2.59	0.48
1:D:193:VAL:CG2	1:D:266:LEU:CD2	2.92	0.47
1:A:164:ARG:HD3	1:A:226:TYR:CE1	2.49	0.47
1:A:254:ASP:CA	1:A:259:VAL:HG12	2.44	0.47
1:C:154:LYS:O	1:C:154:LYS:HG2	2.15	0.47
1:A:79:TRP:CD1	1:A:321:VAL:HA	2.50	0.47
1:A:189:PHE:HB2	1:A:261:HIS:NE2	2.30	0.46
1:B:201:ARG:CZ	1:B:236:LYS:HE2	2.45	0.46
1:D:63:VAL:HA	1:D:66:ARG:NH1	2.31	0.46
1:B:48:ARG:CZ	1:B:89:VAL:HG21	2.46	0.45
1:C:79:TRP:CD1	1:C:321:VAL:HA	2.51	0.45
1:B:25:PRO:CD	1:B:279:VAL:HG22	2.46	0.45
1:C:201:ARG:HH11	1:C:201:ARG:CG	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:PHE:CD1	1:D:99:PHE:C	2.88	0.45
1:C:349:MET:HB2	1:C:349:MET:HE2	1.64	0.45
1:A:279:VAL:HG13	1:A:280:ASP:N	2.31	0.45
1:B:264:MET:O	1:B:268:MET:HG3	2.16	0.45
1:D:164:ARG:HD3	1:D:226:TYR:CE1	2.52	0.45
1:B:176:LEU:O	1:B:180:VAL:HG23	2.18	0.44
1:D:90:MET:HE3	1:D:215:TYR:CD2	2.52	0.44
1:A:286:VAL:O	1:A:289:CYS:HB2	2.17	0.43
1:D:134:ARG:NH2	1:D:151:ASP:OD2	2.44	0.43
1:C:98:VAL:CG1	1:C:99:PHE:N	2.79	0.43
1:C:254:ASP:CB	1:C:259:VAL:CG1	2.92	0.43
1:B:153:LEU:HD13	1:B:153:LEU:O	2.18	0.43
1:A:300:LEU:HD21	1:A:311:VAL:HG11	2.00	0.43
1:B:79:TRP:CD1	1:B:321:VAL:HA	2.53	0.43
1:C:204:ILE:HG23	1:C:206:VAL:H	1.85	0.42
1:D:200:ARG:HA	1:D:200:ARG:HD3	1.82	0.42
1:D:259:VAL:HG22	1:D:260:ASP:N	2.34	0.42
1:D:90:MET:HE2	1:D:215:TYR:CZ	2.55	0.42
1:A:254:ASP:HB3	1:A:259:VAL:CG1	2.50	0.42
1:D:204:ILE:HD12	1:D:206:VAL:CG2	2.49	0.42
1:B:164:ARG:HD3	1:B:226:TYR:CE1	2.54	0.42
1:C:95:ASN:C	1:C:98:VAL:HG12	2.39	0.42
1:B:90:MET:HE3	1:B:215:TYR:CD2	2.55	0.42
1:B:328:TRP:CZ3	1:B:334:ARG:HD2	2.55	0.41
1:C:164:ARG:HD3	1:C:226:TYR:CE1	2.54	0.41
1:D:306:LYS:HD3	1:D:306:LYS:HA	1.64	0.41
1:D:253:LYS:O	1:D:257:LEU:HB2	2.20	0.41
1:C:266:LEU:HD23	1:C:266:LEU:O	2.20	0.41
1:D:328:TRP:CH2	1:D:334:ARG:HD2	2.56	0.41
1:B:204:ILE:HG23	1:B:206:VAL:H	1.85	0.41
1:C:328:TRP:CH2	1:C:334:ARG:HD2	2.56	0.41
1:D:276:GLN:NE2	1:D:280:ASP:OD1	2.54	0.41
1:A:193:VAL:HG22	1:A:266:LEU:HD22	2.02	0.41
1:A:279:VAL:CG1	1:A:280:ASP:N	2.84	0.40
1:D:276:GLN:HA	1:D:279:VAL:HG12	2.03	0.40
1:C:98:VAL:HG13	1:C:99:PHE:H	1.84	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	332/366 (91%)	328 (99%)	4 (1%)	0	100 100
1	B	319/366 (87%)	315 (99%)	4 (1%)	0	100 100
1	C	322/366 (88%)	317 (98%)	5 (2%)	0	100 100
1	D	307/366 (84%)	301 (98%)	6 (2%)	0	100 100
All	All	1280/1464 (87%)	1261 (98%)	19 (2%)	0	100 100

There are no Ramachandran outliers to report.

### 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	287/314 (91%)	286 (100%)	1 (0%)	92 95
1	B	279/314 (89%)	278 (100%)	1 (0%)	91 93
1	C	280/314 (89%)	279 (100%)	1 (0%)	91 93
1	D	272/314 (87%)	272 (100%)	0	100 100
All	All	1118/1256 (89%)	1115 (100%)	3 (0%)	92 95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	TYR
1	B	247	ASP
1	C	90	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	175	GLN
1	A	182	GLN
1	A	220	ASN
1	B	179	GLN
1	B	183	GLN
1	B	287	ASN

### 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 monosaccharides 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 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	334/366 (91%)	-0.39	5 (1%) 73 72	11, 20, 39, 50	0
1	B	325/366 (88%)	-0.33	12 (3%) 41 41	9, 17, 41, 69	0
1	C	326/366 (89%)	-0.10	25 (7%) 13 12	11, 21, 51, 79	0
1	D	318/366 (86%)	0.29	37 (11%) 4 4	13, 27, 68, 87	0
All	All	1303/1464 (89%)	-0.14	79 (6%) 21 20	9, 21, 50, 87	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	269	GLN	4.3
1	D	21	PHE	4.3
1	D	256	GLU	4.2
1	C	259	VAL	4.1
1	D	185	GLY	4.1
1	D	342	GLU	4.1
1	D	132	ALA	4.0
1	D	341	HIS	4.0
1	D	340	GLY	4.0
1	B	185	GLY	3.9
1	C	350	TYR	3.8
1	D	259	VAL	3.8
1	D	114	PRO	3.7
1	D	336	LEU	3.7
1	C	338	PRO	3.6
1	D	252	ARG	3.6
1	C	256	GLU	3.6
1	D	180	VAL	3.6
1	C	257	LEU	3.5
1	D	266	LEU	3.5
1	D	346	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	131	ASN	3.4
1	D	261	HIS	3.3
1	D	184	VAL	3.3
1	D	117	ALA	3.3
1	D	257	LEU	3.2
1	B	20	PRO	3.2
1	D	267	LEU	3.2
1	B	339	GLU	3.2
1	B	259	VAL	3.2
1	C	339	GLU	3.1
1	B	184	VAL	3.0
1	A	260	ASP	3.0
1	C	341	HIS	3.0
1	C	138	GLU	3.0
1	A	352	PRO	3.0
1	C	351	LEU	2.9
1	D	260	ASP	2.9
1	C	20	PRO	2.9
1	B	269	GLN	2.9
1	D	23	ARG	2.9
1	D	196	TYR	2.9
1	C	255	LEU	2.9
1	D	337	GLY	2.9
1	C	261	HIS	2.8
1	D	183	GLN	2.8
1	B	350	TYR	2.8
1	C	184	VAL	2.7
1	D	22	VAL	2.7
1	C	59	PHE	2.7
1	D	333	GLY	2.7
1	C	61	LYS	2.7
1	B	256	GLU	2.6
1	D	349	MET	2.6
1	D	194	GLU	2.6
1	C	58	ASN	2.6
1	B	260	ASP	2.6
1	D	273	LEU	2.5
1	A	259	VAL	2.5
1	A	191	ARG	2.4
1	B	258	GLY	2.4
1	C	337	GLY	2.4
1	B	261	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	66	ARG	2.4
1	D	268	MET	2.4
1	D	182	GLN	2.4
1	C	51	ARG	2.4
1	C	55	ARG	2.3
1	C	98	VAL	2.3
1	C	183	GLN	2.3
1	B	348	ILE	2.2
1	C	63	VAL	2.2
1	D	118	ALA	2.2
1	D	107	GLU	2.1
1	C	345	GLU	2.1
1	D	343	VAL	2.1
1	C	185	GLY	2.1
1	A	272	ASN	2.0
1	D	335	TYR	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 monosaccharides 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.