



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2021 – 08:02 AM EDT

PDB ID : 7S09  
Title : Crystal structure of *Penicillium verruculosum* copalyl diphosphate synthase (PvCPS) alpha prenyltransferase domain variant, F760A  
Authors : Ronnebaum, T.A.; Christianson, D.W.  
Deposited on : 2021-08-30  
Resolution : 3.10 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	:	2.23.2
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)	:	2.23.2

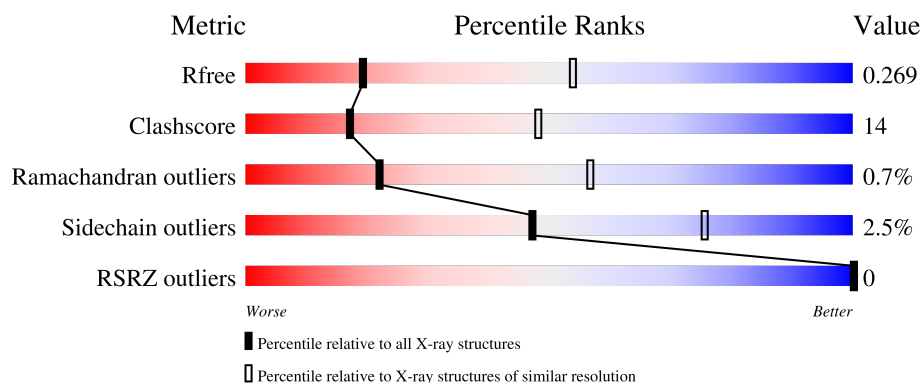
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	305	 70% 28% ..
1	B	305	 61% 35% ..

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4706 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 Terpene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2372	1508	398	453	13			
1	B	296	Total	C	N	O	S	0	0	0
			2334	1488	392	441	13			

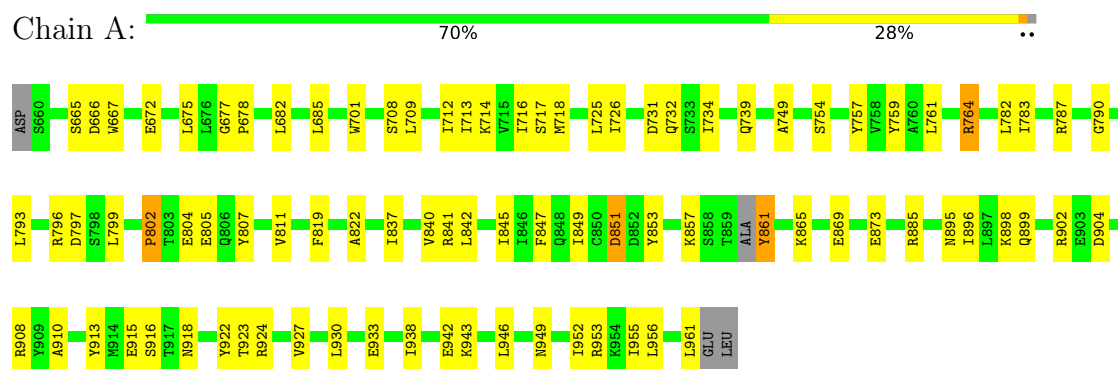
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	760	ALA	PHE	engineered mutation	UNP A0A348FUE1
B	760	ALA	PHE	engineered mutation	UNP A0A348FUE1

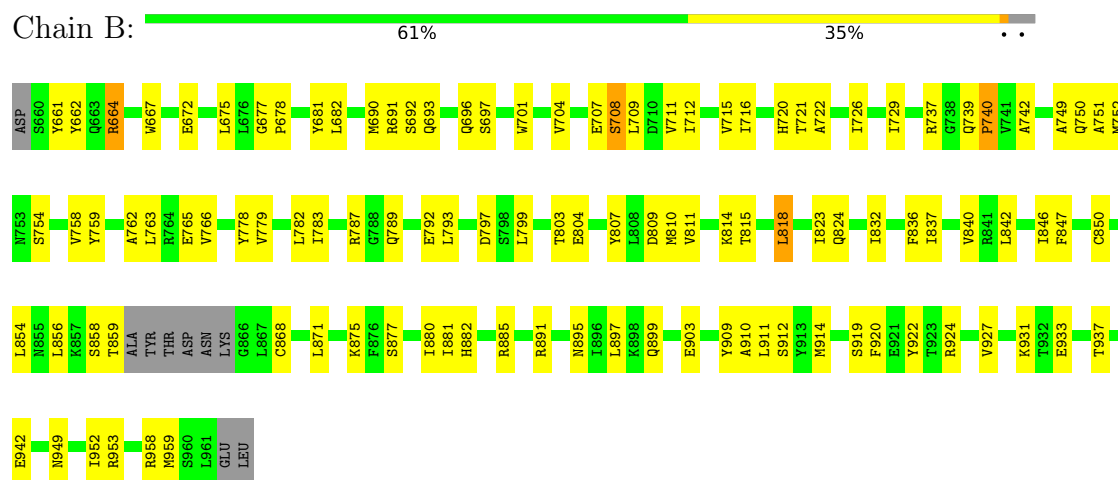
### 3 Residue-property plots

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: Terpene synthase



#### • Molecule 1: Terpene synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.75Å 187.75Å 56.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.87 – 3.10 93.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (93.87-3.10) 93.7 (93.87-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.199 , 0.255 0.210 , 0.269	Depositor DCC
$R_{free}$ test set	1994 reflections (9.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.957	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , -9.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.44	0/2412	0.65	0/3266
1	B	0.44	0/2374	0.65	0/3212
All	All	0.44	0/4786	0.65	0/6478

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

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	2372	0	2349	57	2
1	B	2334	0	2334	82	2
All	All	4706	0	4683	130	2

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 14.

All (130) 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:803:THR:HG22	1:B:885:ARG:HH12	1.13	1.08
1:B:690:MET:HE1	1:B:847:PHE:HD1	1.16	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:MET:HE1	1:B:847:PHE:CD1	1.99	0.98
1:B:690:MET:CE	1:B:847:PHE:CD1	2.53	0.91
1:B:690:MET:CE	1:B:847:PHE:HD1	1.90	0.83
1:A:734:ILE:HD11	1:A:902:ARG:HH22	1.44	0.80
1:B:667:TRP:HE1	1:B:672:GLU:HG2	1.45	0.79
1:B:693:GLN:OE1	1:B:958:ARG:NH1	2.19	0.76
1:B:856:LEU:HB3	1:B:911:LEU:HD21	1.69	0.73
1:B:690:MET:HE1	1:B:959:MET:SD	2.30	0.72
1:A:857:LYS:NZ	1:A:915:GLU:OE2	2.22	0.71
1:A:837:ILE:HA	1:A:840:VAL:HG12	1.75	0.69
1:B:891:ARG:O	1:B:895:ASN:ND2	2.25	0.68
1:B:792:GLU:HB2	1:B:810:MET:HE3	1.74	0.68
1:B:716:ILE:HG23	1:B:818:LEU:HD22	1.76	0.67
1:B:690:MET:CE	1:B:959:MET:SD	2.83	0.66
1:B:789:GLN:O	1:B:793:LEU:HD12	1.96	0.65
1:A:819:PHE:HB3	1:A:840:VAL:HG22	1.78	0.64
1:B:690:MET:SD	1:B:847:PHE:CE1	2.91	0.64
1:B:803:THR:CG2	1:B:885:ARG:HH12	2.02	0.63
1:A:667:TRP:HE1	1:A:672:GLU:HG2	1.63	0.62
1:A:764:ARG:HB2	1:B:779:VAL:HG11	1.81	0.62
1:B:933:GLU:O	1:B:937:THR:OG1	2.13	0.62
1:A:667:TRP:CD2	1:B:787:ARG:HD3	2.35	0.61
1:A:841:ARG:O	1:A:845:ILE:HD12	2.01	0.61
1:B:682:LEU:O	1:B:737:ARG:NH1	2.34	0.60
1:A:665:SER:OG	1:B:809:ASP:OD2	2.19	0.60
1:A:749:ALA:HB1	1:B:793:LEU:HD22	1.82	0.60
1:A:913:TYR:O	1:A:916:SER:OG	2.15	0.60
1:B:722:ALA:O	1:B:726:ILE:HG13	2.01	0.60
1:B:877:SER:O	1:B:881:ILE:HG13	2.02	0.59
1:B:681:TYR:OH	1:B:740:PRO:O	2.15	0.59
1:B:704:VAL:HB	1:B:709:LEU:HD13	1.85	0.59
1:A:797:ASP:OD2	1:B:750:GLN:HG3	2.03	0.58
1:A:716:ILE:HG13	1:A:822:ALA:HB2	1.85	0.58
1:B:842:LEU:HD21	1:B:933:GLU:HB3	1.85	0.58
1:A:952:ILE:HD12	1:A:955:ILE:HD11	1.86	0.57
1:B:803:THR:HG22	1:B:885:ARG:NH1	1.98	0.57
1:B:836:PHE:O	1:B:840:VAL:HG23	2.04	0.57
1:A:853:TYR:OH	1:A:924:ARG:NH1	2.38	0.56
1:A:807:TYR:O	1:A:811:VAL:HG23	2.04	0.56
1:B:701:TRP:CZ2	1:B:949:ASN:HB2	2.39	0.56
1:B:903:GLU:OE1	1:B:903:GLU:N	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:GLU:OE2	1:B:922:TYR:OH	2.20	0.55
1:B:711:VAL:O	1:B:715:VAL:HG13	2.07	0.55
1:A:667:TRP:NE1	1:A:672:GLU:HG2	2.22	0.54
1:B:850:CYS:O	1:B:854:LEU:HG	2.07	0.53
1:B:807:TYR:O	1:B:811:VAL:HG23	2.08	0.53
1:B:882:HIS:ND1	1:B:919:SER:HB3	2.24	0.53
1:A:802:PRO:O	1:A:885:ARG:NE	2.33	0.53
1:A:790:GLY:HA3	1:B:675:LEU:HD21	1.91	0.52
1:B:762:ALA:O	1:B:766:VAL:HG23	2.09	0.51
1:B:692:SER:O	1:B:696:GLN:HG2	2.11	0.51
1:A:799:LEU:HD11	1:A:898:LYS:HB2	1.93	0.50
1:A:923:THR:O	1:A:927:VAL:HG23	2.11	0.50
1:B:810:MET:HG3	1:B:811:VAL:N	2.25	0.50
1:A:930:LEU:HD21	1:B:661:TYR:HD2	1.75	0.50
1:B:803:THR:HA	1:B:885:ARG:NH1	2.27	0.50
1:B:909:TYR:O	1:B:912:SER:HB3	2.11	0.50
1:A:845:ILE:O	1:A:849:ILE:HG13	2.11	0.50
1:A:851:ASP:OD1	1:A:861:TYR:OH	2.29	0.50
1:B:868:CYS:HB3	1:B:871:LEU:HD12	1.94	0.49
1:B:715:VAL:HG12	1:B:765:GLU:HB3	1.95	0.49
1:B:880:ILE:HG21	1:B:897:LEU:HD11	1.93	0.49
1:B:678:PRO:HG2	1:B:751:ALA:HA	1.94	0.49
1:B:682:LEU:HD13	1:B:742:ALA:HB2	1.95	0.49
1:B:739:GLN:HB3	1:B:740:PRO:HD2	1.94	0.49
1:B:690:MET:SD	1:B:847:PHE:HE1	2.34	0.48
1:B:782:LEU:HA	1:B:782:LEU:HD13	1.66	0.48
1:A:672:GLU:OE2	1:A:757:TYR:OH	2.20	0.48
1:A:942:GLU:HA	1:A:946:LEU:HB2	1.94	0.48
1:A:904:ASP:O	1:A:908:ARG:HG3	2.13	0.48
1:B:682:LEU:HB3	1:B:721:THR:HG23	1.96	0.48
1:B:675:LEU:O	1:B:754:SER:OG	2.25	0.48
1:B:832:ILE:N	1:B:832:ILE:HD12	2.28	0.48
1:B:690:MET:SD	1:B:847:PHE:CD1	3.07	0.47
1:A:805:GLU:H	1:A:805:GLU:CD	2.17	0.47
1:B:690:MET:HE3	1:B:959:MET:SD	2.53	0.47
1:B:792:GLU:OE1	1:B:810:MET:HE1	2.14	0.47
1:B:708:SER:O	1:B:712:ILE:HG13	2.15	0.47
1:A:793:LEU:HD22	1:B:749:ALA:HB1	1.95	0.46
1:A:938:ILE:HD13	1:A:952:ILE:HG23	1.97	0.46
1:A:896:ILE:HD13	1:A:910:ALA:HB2	1.97	0.46
1:B:783:ILE:O	1:B:787:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ILE:HD12	1:A:759:TYR:HE2	1.80	0.46
1:B:799:LEU:HD13	1:B:799:LEU:HA	1.72	0.46
1:A:712:ILE:O	1:A:716:ILE:HG12	2.15	0.46
1:A:955:ILE:HG13	1:A:956:LEU:N	2.31	0.45
1:A:682:LEU:HD22	1:A:725:LEU:HG	1.97	0.45
1:A:731:ASP:O	1:A:732:GLN:HB2	2.17	0.45
1:A:804:GLU:OE2	1:A:922:TYR:OH	2.24	0.45
1:A:761:LEU:HA	1:A:761:LEU:HD23	1.78	0.45
1:A:847:PHE:O	1:A:851:ASP:HB2	2.17	0.45
1:A:726:ILE:HG23	1:B:752:MET:HE1	2.00	0.45
1:B:662:TYR:CZ	1:B:664:ARG:HA	2.53	0.44
1:B:729:ILE:HD13	1:B:752:MET:HB2	2.00	0.44
1:B:920:PHE:O	1:B:924:ARG:HG3	2.17	0.44
1:B:691:ARG:HD2	1:B:720:HIS:CG	2.53	0.43
1:A:685:LEU:CD1	1:A:739:GLN:HB2	2.49	0.43
1:A:714:LYS:HG2	1:A:718:MET:SD	2.58	0.43
1:A:677:GLY:H	1:A:678:PRO:CD	2.31	0.43
1:B:842:LEU:O	1:B:846:ILE:HG13	2.18	0.43
1:A:796:ARG:HD2	1:A:873:GLU:O	2.18	0.43
1:A:677:GLY:H	1:A:678:PRO:HD2	1.84	0.43
1:B:763:LEU:HD13	1:B:778:TYR:CE1	2.54	0.43
1:B:823:ILE:HG13	1:B:840:VAL:HG21	2.00	0.43
1:B:927:VAL:O	1:B:931:LYS:HG3	2.19	0.42
1:A:895:ASN:O	1:A:899:GLN:HG2	2.19	0.42
1:A:949:ASN:HB3	1:A:952:ILE:CG2	2.49	0.42
1:B:824:GLN:HG3	1:B:837:ILE:CD1	2.50	0.42
1:B:910:ALA:O	1:B:914:MET:HG3	2.19	0.42
1:B:942:GLU:OE1	1:B:953:ARG:NH2	2.33	0.42
1:A:675:LEU:HD12	1:A:757:TYR:CD2	2.54	0.42
1:B:707:GLU:O	1:B:711:VAL:HG23	2.19	0.42
1:A:961:LEU:HD23	1:A:961:LEU:HA	1.75	0.41
1:B:895:ASN:O	1:B:899:GLN:HG2	2.20	0.41
1:B:754:SER:O	1:B:758:VAL:HG23	2.21	0.41
1:B:875:LYS:HG2	1:B:877:SER:HB3	2.02	0.41
1:B:667:TRP:CZ2	1:B:675:LEU:HD12	2.55	0.41
1:B:814:LYS:HG3	1:B:815:THR:N	2.36	0.41
1:A:708:SER:O	1:A:712:ILE:HG13	2.20	0.41
1:A:783:ILE:O	1:A:787:ARG:HG3	2.21	0.41
1:B:858:SER:O	1:B:859:THR:OG1	2.36	0.41
1:A:949:ASN:HB3	1:A:952:ILE:HG21	2.03	0.40
1:A:952:ILE:HD12	1:A:952:ILE:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:TRP:HZ2	1:A:942:GLU:HG3	1.87	0.40
1:A:842:LEU:HD21	1:A:933:GLU:HB3	2.03	0.40
1:B:949:ASN:OD1	1:B:952:ILE:HB	2.21	0.40
1:A:709:LEU:O	1:A:713:ILE:HG13	2.21	0.40
1:A:865:LYS:O	1:A:869:GLU:HB2	2.21	0.40

All (2) 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:918:ASN:OD1	1:B:924:ARG:NH2[2_664]	2.07	0.13
1:A:898:LYS:NZ	1:B:797:ASP:O[2_665]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	297/305 (97%)	263 (89%)	32 (11%)	2 (1%)	22	57
1	B	292/305 (96%)	269 (92%)	21 (7%)	2 (1%)	22	57
All	All	589/610 (97%)	532 (90%)	53 (9%)	4 (1%)	22	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	677	GLY
1	B	664	ARG
1	A	943	LYS
1	A	802	PRO

### 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	259/272 (95%)	251 (97%)	8 (3%)	40	70
1	B	256/272 (94%)	251 (98%)	5 (2%)	55	80
All	All	515/544 (95%)	502 (98%)	13 (2%)	47	75

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

Mol	Chain	Res	Type
1	A	666	ASP
1	A	717	SER
1	A	754	SER
1	A	764	ARG
1	A	782	LEU
1	A	851	ASP
1	A	861	TYR
1	A	953	ARG
1	B	697	SER
1	B	708	SER
1	B	740	PRO
1	B	759	TYR
1	B	818	LEU

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

### 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 [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	301/305 (98%)	-0.27	0 100 100	8, 18, 40, 53	0
1	B	296/305 (97%)	-0.30	0 100 100	7, 18, 38, 45	0
All	All	597/610 (97%)	-0.29	0 100 100	7, 18, 40, 53	0

There are no RSRZ outliers to report.

### 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.