Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2016 – 05:14 PM EDT

PDB ID	:	5ERF
Title	:	Ketosynthase from module 6 of the bacillaene synthase from Bacillus subtilis 168
Authors	:	Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.
Deposited on	:	2015-11-14
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*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

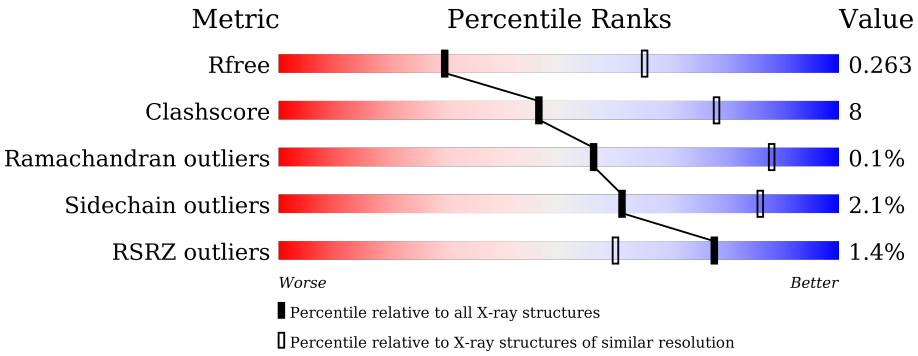
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 >=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 <=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	617	2% 76% 12% • 10%
1	B	617	% 78% 12% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8719 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 Polyketide synthase PksL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4329	2748	726	829	26			
1	B	560	Total	C	N	O	S	0	0	0
			4390	2789	734	840	27			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q05470
A	-20	GLY	-	expression tag	UNP Q05470
A	-19	SER	-	expression tag	UNP Q05470
A	-18	SER	-	expression tag	UNP Q05470
A	-17	HIS	-	expression tag	UNP Q05470
A	-16	HIS	-	expression tag	UNP Q05470
A	-15	HIS	-	expression tag	UNP Q05470
A	-14	HIS	-	expression tag	UNP Q05470
A	-13	HIS	-	expression tag	UNP Q05470
A	-12	HIS	-	expression tag	UNP Q05470
A	-11	SER	-	expression tag	UNP Q05470
A	-10	SER	-	expression tag	UNP Q05470
A	-9	GLY	-	expression tag	UNP Q05470
A	-8	LEU	-	expression tag	UNP Q05470
A	-7	VAL	-	expression tag	UNP Q05470
A	-6	PRO	-	expression tag	UNP Q05470
A	-5	ARG	-	expression tag	UNP Q05470
A	-4	GLY	-	expression tag	UNP Q05470
A	-3	SER	-	expression tag	UNP Q05470
A	-2	SER	-	expression tag	UNP Q05470
B	-21	MET	-	initiating methionine	UNP Q05470
B	-20	GLY	-	expression tag	UNP Q05470
B	-19	SER	-	expression tag	UNP Q05470
B	-18	SER	-	expression tag	UNP Q05470
B	-17	HIS	-	expression tag	UNP Q05470

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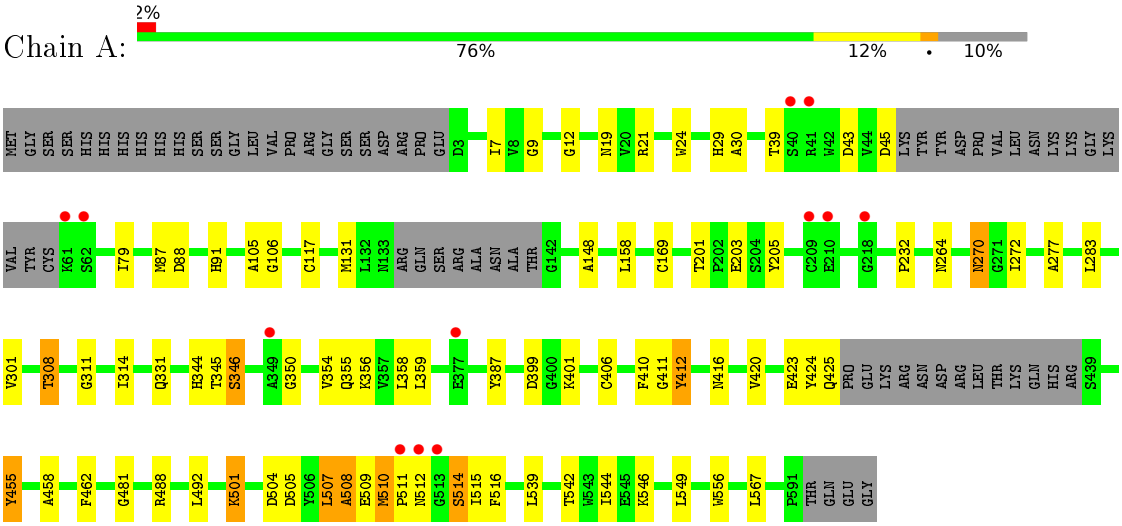
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q05470
B	-15	HIS	-	expression tag	UNP Q05470
B	-14	HIS	-	expression tag	UNP Q05470
B	-13	HIS	-	expression tag	UNP Q05470
B	-12	HIS	-	expression tag	UNP Q05470
B	-11	SER	-	expression tag	UNP Q05470
B	-10	SER	-	expression tag	UNP Q05470
B	-9	GLY	-	expression tag	UNP Q05470
B	-8	LEU	-	expression tag	UNP Q05470
B	-7	VAL	-	expression tag	UNP Q05470
B	-6	PRO	-	expression tag	UNP Q05470
B	-5	ARG	-	expression tag	UNP Q05470
B	-4	GLY	-	expression tag	UNP Q05470
B	-3	SER	-	expression tag	UNP Q05470
B	-2	SER	-	expression tag	UNP Q05470

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.

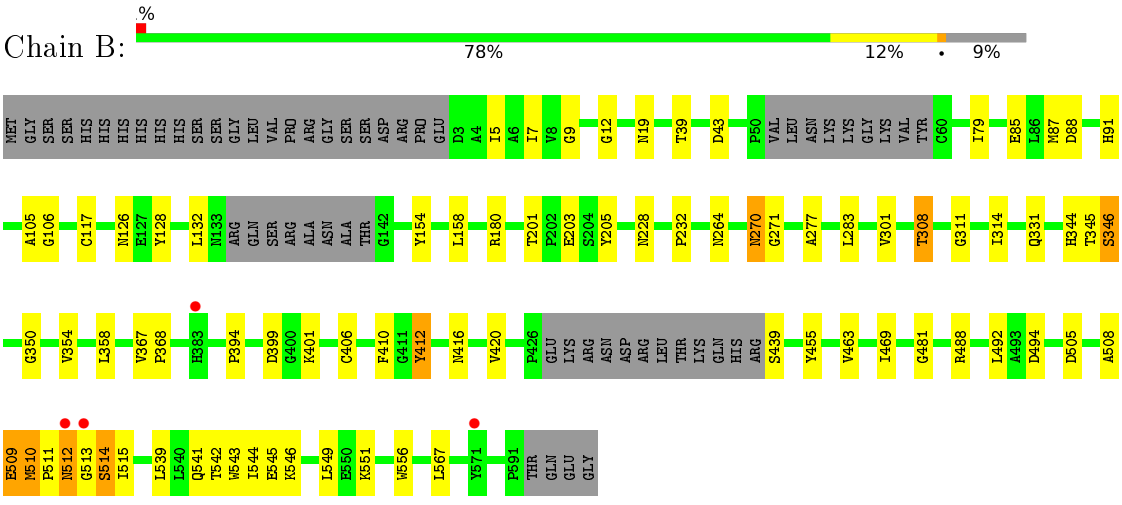
- Molecule 1: Polyketide synthase PksL

Chain A:



- Molecule 1: Polyketide synthase PksL

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.06Å 77.32Å 85.29Å 77.91° 70.26° 64.18°	Depositor
Resolution (Å)	39.73 – 3.10 39.73 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (39.73-3.10) 92.2 (39.73-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.219 , 0.268 0.218 , 0.263	Depositor DCC
R_{free} test set	1285 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8719	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.42	0/4424	0.68	6/5982 (0.1%)
1	B	0.42	0/4489	0.76	9/6072 (0.1%)
All	All	0.42	0/8913	0.72	15/12054 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	512	ASN	CB-CA-C	-19.43	71.54	110.40
1	B	514	SER	CB-CA-C	10.14	129.37	110.10
1	B	510	MET	CB-CA-C	-8.71	92.97	110.40
1	B	510	MET	N-CA-C	8.44	133.77	111.00
1	B	515	ILE	N-CA-C	8.28	133.35	111.00
1	A	507	LEU	CB-CA-C	-7.02	96.85	110.20
1	A	501	LYS	CB-CA-C	-6.71	96.97	110.40
1	B	512	ASN	N-CA-C	6.17	127.66	111.00
1	A	508	ALA	N-CA-C	-5.91	95.03	111.00
1	A	507	LEU	N-CA-C	5.83	126.74	111.00
1	A	508	ALA	N-CA-CB	5.76	118.16	110.10
1	B	515	ILE	N-CA-CB	-5.32	98.56	110.80
1	A	515	ILE	N-CA-CB	5.20	122.75	110.80
1	B	271	GLY	N-CA-C	-5.16	100.19	113.10
1	B	514	SER	N-CA-C	-5.03	97.43	111.00

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	4329	0	4235	77	3
1	B	4390	0	4289	55	3
All	All	8719	0	8524	131	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 8.

All (131) 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:505:ASP:HB3	1:B:511:PRO:CG	1.34	1.54
1:B:505:ASP:CB	1:B:511:PRO:CG	2.18	1.20
1:A:505:ASP:CB	1:A:511:PRO:HB3	1.69	1.20
1:A:505:ASP:HB3	1:A:511:PRO:HB3	1.17	1.11
1:B:505:ASP:HB3	1:B:511:PRO:HG2	1.22	1.10
1:A:505:ASP:HB3	1:A:511:PRO:CB	1.81	1.09
1:B:505:ASP:HB3	1:B:511:PRO:CD	1.82	1.09
1:B:505:ASP:CB	1:B:511:PRO:HG3	1.84	1.05
1:B:505:ASP:CG	1:B:511:PRO:HG3	1.79	1.02
1:A:43:ASP:OD1	1:A:45:ASP:N	2.00	0.93
1:B:505:ASP:HB3	1:B:511:PRO:HG3	1.39	0.90
1:B:505:ASP:CB	1:B:511:PRO:HG2	1.96	0.85
1:A:131:MET:HE2	1:A:201:THR:HG22	1.61	0.81
1:A:505:ASP:CG	1:A:511:PRO:HA	2.09	0.72
1:A:331:GLN:OE1	1:A:387:TYR:HB3	1.88	0.72
1:A:492:LEU:HD21	1:A:549:LEU:HB2	1.75	0.69
1:B:399:ASP:HB2	1:B:401:LYS:HG2	1.76	0.68
1:B:492:LEU:HD21	1:B:549:LEU:HB2	1.75	0.67
1:A:399:ASP:HB2	1:A:401:LYS:HG2	1.76	0.66
1:B:505:ASP:OD2	1:B:511:PRO:HG3	1.95	0.66
1:A:270:ASN:ND2	1:A:270:ASN:O	2.28	0.66
1:A:505:ASP:CG	1:A:511:PRO:HB3	2.15	0.66
1:A:510:MET:N	1:A:511:PRO:CD	2.59	0.65
1:A:131:MET:HE2	1:A:201:THR:CG2	2.27	0.65
1:A:131:MET:CE	1:A:201:THR:CG2	2.75	0.64
1:A:301:VAL:HG22	1:A:406:CYS:HB2	1.79	0.64
1:B:301:VAL:HG22	1:B:406:CYS:HB2	1.80	0.64
1:B:88:ASP:HB3	1:B:91:HIS:CD2	2.33	0.64
1:B:270:ASN:O	1:B:270:ASN:ND2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ASP:HB3	1:A:511:PRO:CG	2.29	0.62
1:A:7:ILE:HD13	1:A:358:LEU:HD11	1.82	0.62
1:A:501:LYS:O	1:A:501:LYS:CG	2.46	0.61
1:B:7:ILE:HD13	1:B:358:LEU:HD11	1.82	0.61
1:A:504:ASP:O	1:A:507:LEU:HB2	2.01	0.61
1:A:88:ASP:HB3	1:A:91:HIS:CD2	2.37	0.60
1:A:455:TYR:O	1:A:458:ALA:HB3	2.02	0.60
1:A:510:MET:N	1:A:511:PRO:HD3	2.16	0.59
1:B:544:ILE:HG23	1:B:567:LEU:HD12	1.84	0.59
1:A:505:ASP:CG	1:A:511:PRO:CA	2.71	0.59
1:A:544:ILE:HG23	1:A:567:LEU:HD12	1.84	0.58
1:A:131:MET:HE3	1:A:201:THR:HG23	1.84	0.58
1:A:79:ILE:HG21	1:A:87:MET:HE3	1.85	0.58
1:B:505:ASP:CB	1:B:511:PRO:CD	2.69	0.57
1:A:542:THR:O	1:A:546:LYS:HB2	2.03	0.57
1:A:492:LEU:HD12	1:A:492:LEU:N	2.19	0.57
1:A:505:ASP:CB	1:A:511:PRO:CB	2.54	0.57
1:B:492:LEU:HD12	1:B:492:LEU:N	2.19	0.57
1:A:508:ALA:O	1:A:509:GLU:HG2	2.05	0.56
1:A:505:ASP:O	1:A:509:GLU:HA	2.06	0.56
1:B:546:LYS:O	1:B:546:LYS:HG2	2.05	0.56
1:B:205:TYR:CZ	1:B:232:PRO:HG2	2.43	0.53
1:B:79:ILE:HG21	1:B:87:MET:HE3	1.89	0.53
1:A:424:TYR:CG	1:A:425:GLN:N	2.77	0.53
1:B:264:ASN:ND2	1:B:283:LEU:HB2	2.23	0.53
1:B:201:THR:HB	1:B:203:GLU:OE2	2.08	0.53
1:A:201:THR:HB	1:A:203:GLU:OE2	2.08	0.52
1:B:512:ASN:N	1:B:513:GLY:HA2	2.25	0.52
1:A:516:PHE:CD1	1:A:516:PHE:N	2.76	0.52
1:B:512:ASN:N	1:B:513:GLY:CA	2.73	0.51
1:A:205:TYR:CZ	1:A:232:PRO:HG2	2.45	0.51
1:A:406:CYS:SG	1:A:420:VAL:HG22	2.51	0.51
1:B:308:THR:CG2	1:B:311:GLY:HA3	2.41	0.51
1:B:12:GLY:O	1:B:19:ASN:HA	2.10	0.51
1:A:264:ASN:ND2	1:A:283:LEU:HB2	2.25	0.51
1:B:308:THR:HG23	1:B:311:GLY:H	1.75	0.50
1:B:505:ASP:HB3	1:B:511:PRO:HD3	1.82	0.50
1:A:12:GLY:O	1:A:19:ASN:HA	2.10	0.50
1:A:308:THR:CG2	1:A:311:GLY:HA3	2.42	0.50
1:A:505:ASP:CG	1:A:511:PRO:CB	2.78	0.49
1:A:508:ALA:O	1:A:510:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:CYS:SG	1:B:420:VAL:HG22	2.52	0.49
1:B:277:ALA:HB2	1:B:314:ILE:HG23	1.93	0.49
1:B:39:THR:HG22	1:B:43:ASP:HA	1.94	0.49
1:A:308:THR:HG23	1:A:311:GLY:H	1.77	0.49
1:A:39:THR:HG22	1:A:43:ASP:HA	1.94	0.49
1:A:508:ALA:C	1:A:509:GLU:HG2	2.32	0.48
1:A:9:GLY:HA3	1:A:105:ALA:HB2	1.96	0.48
1:A:43:ASP:OD1	1:A:45:ASP:HB2	2.14	0.48
1:A:455:TYR:O	1:A:458:ALA:N	2.46	0.48
1:A:505:ASP:O	1:A:509:GLU:CA	2.62	0.48
1:A:508:ALA:O	1:A:509:GLU:CG	2.62	0.48
1:A:277:ALA:HB2	1:A:314:ILE:HG23	1.95	0.48
1:A:344:HIS:CD2	1:A:346:SER:H	2.32	0.47
1:B:9:GLY:HA3	1:B:105:ALA:HB2	1.95	0.47
1:B:344:HIS:CD2	1:B:346:SER:H	2.33	0.47
1:B:539:LEU:O	1:B:542:THR:HB	2.14	0.46
1:A:117:CYS:HB3	1:A:158:LEU:HD13	1.96	0.46
1:A:350:GLY:O	1:A:354:VAL:HG23	2.15	0.46
1:A:505:ASP:HB3	1:A:511:PRO:CD	2.44	0.46
1:B:510:MET:HB2	1:B:511:PRO:HD3	1.97	0.46
1:A:410:PHE:HD1	1:A:416:ASN:HB3	1.81	0.46
1:A:539:LEU:O	1:A:542:THR:HB	2.16	0.46
1:A:344:HIS:HD2	1:A:346:SER:H	1.64	0.46
1:A:423:GLU:HG2	1:A:424:TYR:O	2.15	0.45
1:B:132:LEU:HA	1:B:132:LEU:HD23	1.82	0.45
1:A:21:ARG:HE	1:A:462:PHE:HE1	1.63	0.45
1:A:131:MET:HE3	1:A:201:THR:CG2	2.42	0.45
1:A:131:MET:CE	1:A:201:THR:HG23	2.42	0.45
1:A:264:ASN:OD1	1:A:264:ASN:C	2.55	0.45
1:B:505:ASP:CB	1:B:511:PRO:HD3	2.43	0.45
1:B:350:GLY:O	1:B:354:VAL:HG23	2.16	0.45
1:B:117:CYS:HB3	1:B:158:LEU:HD13	1.98	0.45
1:A:169:CYS:HB2	1:A:411:GLY:HA2	1.98	0.44
1:A:412:TYR:CD1	1:A:412:TYR:C	2.91	0.44
1:B:106:GLY:O	1:B:481:GLY:HA2	2.18	0.44
1:B:488:ARG:HB3	1:B:556:TRP:CZ3	2.53	0.44
1:B:344:HIS:HD2	1:B:346:SER:H	1.66	0.43
1:B:508:ALA:O	1:B:509:GLU:HB2	2.18	0.43
1:A:106:GLY:O	1:A:481:GLY:HA2	2.19	0.43
1:B:412:TYR:CD1	1:B:412:TYR:C	2.91	0.43
1:A:488:ARG:HB3	1:A:556:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:PHE:HD1	1:B:416:ASN:HB3	1.84	0.43
1:B:543:TRP:CE2	1:B:551:LYS:CD	3.02	0.43
1:A:501:LYS:O	1:A:501:LYS:HG2	2.19	0.43
1:A:505:ASP:O	1:A:509:GLU:N	2.52	0.42
1:A:91:HIS:CE1	1:A:148:ALA:HB2	2.55	0.42
1:A:505:ASP:OD2	1:A:511:PRO:HA	2.20	0.42
1:A:355:GLN:O	1:A:356:LYS:C	2.57	0.42
1:A:505:ASP:HB3	1:A:511:PRO:CA	2.46	0.42
1:B:463:VAL:HA	1:B:469:ILE:HD11	2.02	0.41
1:B:85:GLU:O	1:B:128:TYR:OH	2.26	0.41
1:B:511:PRO:C	1:B:513:GLY:HA3	2.41	0.41
1:A:410:PHE:CD1	1:A:416:ASN:HB3	2.56	0.41
1:A:24:TRP:HB2	1:A:359:LEU:HD13	2.03	0.41
1:A:29:HIS:O	1:A:30:ALA:C	2.59	0.41
1:B:541:GLN:O	1:B:545:GLU:HB2	2.21	0.41
1:B:439:SER:HA	1:B:494:ASP:HB3	2.03	0.41
1:B:5:ILE:HG13	1:B:180:ARG:HG3	2.04	0.40
1:A:424:TYR:O	1:A:425:GLN:HG3	2.22	0.40
1:B:367:VAL:HB	1:B:368:PRO:CD	2.52	0.40
1:A:272:ILE:HA	1:B:154:TYR:CE1	2.56	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)
1:A:512:ASN:OD1	1:B:394:PRO:CB[1_456]	2.07	0.13
1:A:512:ASN:CG	1:B:394:PRO:CB[1_456]	2.17	0.03
1:A:512:ASN:C	1:B:394:PRO:CG[1_456]	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	545/617 (88%)	505 (93%)	39 (7%)	1 (0%)	52 84
1	B	552/617 (90%)	517 (94%)	35 (6%)	0	100 100
All	All	1097/1234 (89%)	1022 (93%)	74 (7%)	1 (0%)	56 88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	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	458/515 (89%)	450 (98%)	8 (2%)	68 89
1	B	465/515 (90%)	454 (98%)	11 (2%)	57 84
All	All	923/1030 (90%)	904 (98%)	19 (2%)	61 86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	308	THR
1	A	345	THR
1	A	346	SER
1	A	412	TYR
1	A	455	TYR
1	A	510	MET
1	A	514	SER
1	B	126	ASN
1	B	228	ASN
1	B	270	ASN
1	B	308	THR
1	B	331	GLN
1	B	345	THR
1	B	346	SER

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Mol	Chain	Res	Type
1	B	412	TYR
1	B	455	TYR
1	B	509	GLU
1	B	514	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	344	HIS
1	A	378	HIS
1	B	91	HIS
1	B	126	ASN
1	B	344	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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^2)	Q<0.9
1	A	553/617 (89%)	-0.24	12 (2%) 65 42	25, 73, 126, 164	0
1	B	560/617 (90%)	-0.39	4 (0%) 89 78	25, 67, 107, 144	0
All	All	1113/1234 (90%)	-0.32	16 (1%) 78 60	25, 70, 119, 164	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	ASN	6.5
1	B	512	ASN	4.5
1	A	210	GLU	4.3
1	A	511	PRO	3.9
1	A	209	CYS	3.4
1	B	513	GLY	2.9
1	A	40	SER	2.8
1	A	513	GLY	2.7
1	A	61	LYS	2.7
1	A	218	GLY	2.5
1	A	349	ALA	2.3
1	A	62	SER	2.3
1	A	41	ARG	2.2
1	B	571	TYR	2.2
1	B	383	HIS	2.1
1	A	377	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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.