Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:49 AM GMT

PDB ID	:	2IWM
Title	:	PRECURSOR MUTANT CYS1SER OF PENICILLIN V ACYLASE FROM BACILLUS SPHAERICUS
Authors	:	Chandra, P.M.; Dodson, G.; Suresh, C.G.
Deposited on	:	2006-07-01
Resolution	:	2.50 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 (i) symbol.

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

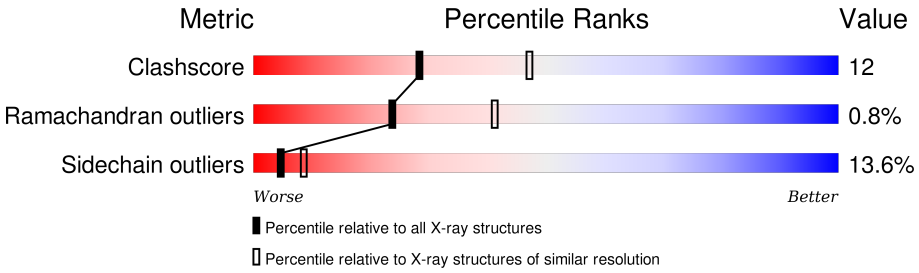
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	74% 19% 5% ••
1	B	338	69% 22% 7% ••
1	C	338	70% 22% 6% ••
1	D	338	67% 24% 7% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10733 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 PENICILLIN ACYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2606	1659	427	507	13			
1	B	334	Total	C	N	O	S	0	0	0
			2606	1659	427	507	13			
1	C	333	Total	C	N	O	S	0	0	0
			2599	1654	426	506	13			
1	D	333	Total	C	N	O	S	0	0	0
			2599	1654	426	506	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	CYS	ENGINEERED MUTATION	UNP P12256
B	4	SER	CYS	ENGINEERED MUTATION	UNP P12256
C	4	SER	CYS	ENGINEERED MUTATION	UNP P12256
D	4	SER	CYS	ENGINEERED MUTATION	UNP P12256
A	101	ARG	THR	CONFLICT	UNP P12256
B	101	ARG	THR	CONFLICT	UNP P12256
C	101	ARG	THR	CONFLICT	UNP P12256
D	101	ARG	THR	CONFLICT	UNP P12256

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	72	Total	O	0	0
			72	72		
2	C	72	Total	O	0	0
			72	72		
2	D	89	Total	O	0	0
			89	89		

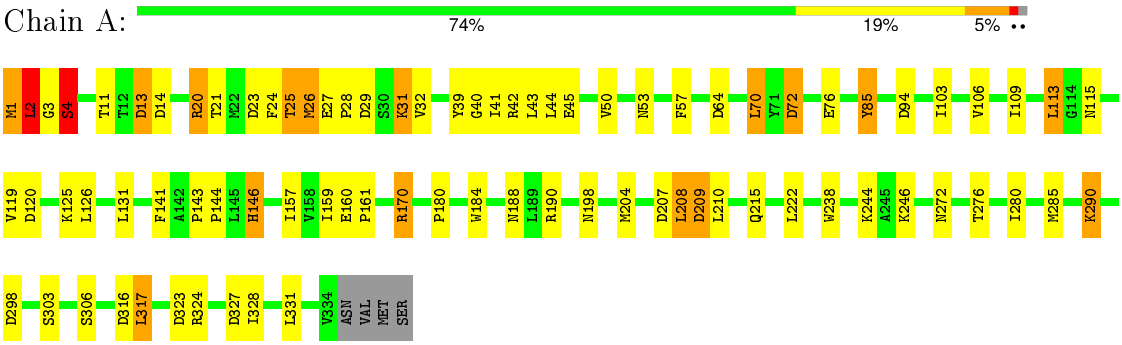
3 Residue-property plots (i)

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.

Note EDS was not executed.

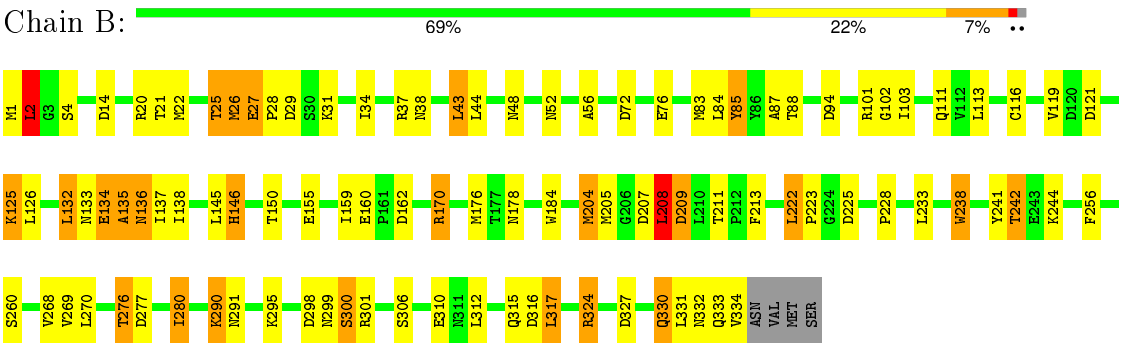
- Molecule 1: PENICILLIN ACYLASE

Chain A:



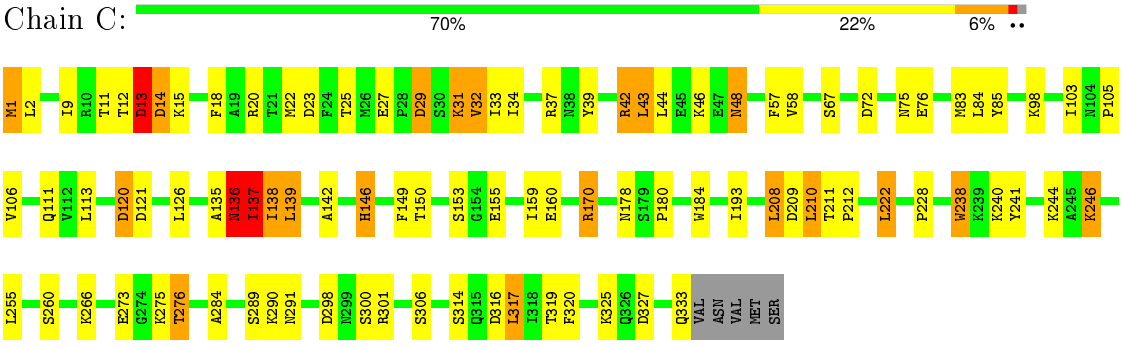
- Molecule 1: PENICILLIN ACYLASE

Chain B:



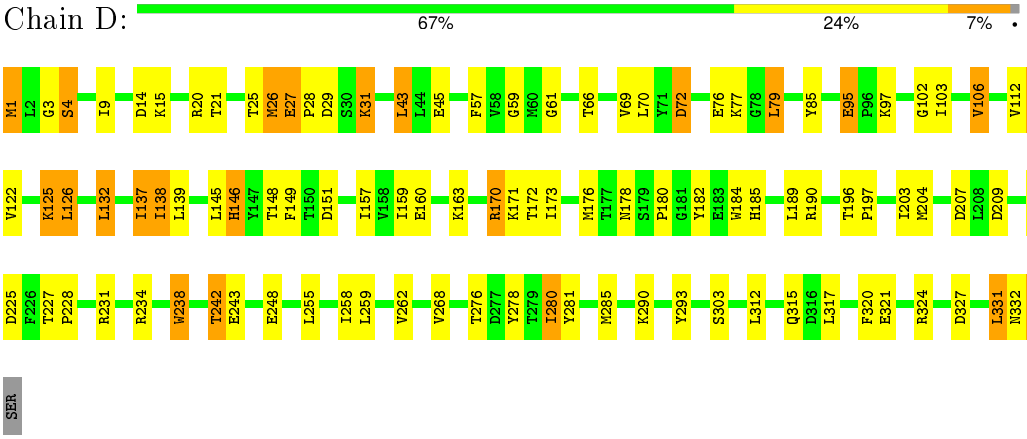
- Molecule 1: PENICILLIN ACYLASE

Chain C:



• Molecule 1: PENICILLIN ACYLASE

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.64Å 90.09Å 102.27Å 90.00° 102.13° 90.00°	Depositor
Resolution (Å)	100.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.8 (100.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.201 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10733	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

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	0.68	0/2661	0.91	12/3616 (0.3%)
1	B	0.64	0/2661	0.91	18/3616 (0.5%)
1	C	0.64	0/2654	0.86	9/3606 (0.2%)
1	D	0.65	0/2654	0.88	8/3606 (0.2%)
All	All	0.65	0/10630	0.89	47/14444 (0.3%)

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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	LEU	O-C-N	-11.19	104.79	122.70
1	A	13	ASP	CB-CG-OD2	8.09	125.58	118.30
1	B	208	LEU	C-N-CA	7.51	140.49	121.70
1	A	72	ASP	CB-CG-OD2	7.43	124.99	118.30
1	C	13	ASP	CB-CG-OD2	7.22	124.79	118.30
1	B	208	LEU	CA-C-N	7.11	132.83	117.20
1	B	209	ASP	O-C-N	7.05	133.99	122.70
1	D	72	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	207	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	327	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	64	ASP	CB-CG-OD2	6.46	124.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	225	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	209	ASP	CA-C-N	-6.12	103.73	117.20
1	A	327	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	23	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	316	ASP	CB-CG-OD2	6.04	123.74	118.30
1	C	298	ASP	CB-CG-OD2	6.01	123.71	118.30
1	C	327	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	120	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	316	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	120	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	162	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	209	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	72	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	207	ASP	CB-CG-OD2	5.81	123.53	118.30
1	D	29	ASP	CB-CG-OD2	5.72	123.45	118.30
1	D	14	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	241	TYR	C-N-CA	-5.63	107.62	121.70
1	B	94	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	23	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	207	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	327	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	151	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	298	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	14	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	29	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	14	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	121	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	72	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	13	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	B	277	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	209	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	14	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	316	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	225	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	121	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	29	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	208	LEU	Peptide
1	C	136	ASN	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	2606	0	2587	51	0
1	B	2606	0	2587	68	0
1	C	2599	0	2578	61	0
1	D	2599	0	2578	75	0
2	A	90	0	0	2	0
2	B	72	0	0	1	0
2	C	72	0	0	0	0
2	D	89	0	0	2	0
All	All	10733	0	10330	241	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 12.

All (241) 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:170:ARG:HH11	1:B:170:ARG:HG3	1.06	1.14
1:A:24:PHE:HB3	1:A:280:ILE:HD11	1.17	1.10
1:A:24:PHE:HB3	1:A:280:ILE:CD1	1.83	1.07
1:C:137:ILE:O	1:C:137:ILE:HG13	1.53	1.03
1:B:134:GLU:O	1:B:135:ALA:CB	2.13	0.95
1:D:95:GLU:OE1	1:D:95:GLU:HA	1.69	0.90
1:B:238:TRP:O	1:B:242:THR:HG23	1.72	0.89
1:A:24:PHE:CB	1:A:280:ILE:HD11	2.03	0.87
1:A:170:ARG:HG2	1:A:170:ARG:HH11	1.39	0.87
1:B:170:ARG:NH1	1:B:170:ARG:HG3	1.78	0.87
1:D:27:GLU:OE1	1:D:324:ARG:HD3	1.74	0.87
1:A:3:GLY:O	1:A:4:SER:OG	1.92	0.87
1:B:238:TRP:O	1:B:242:THR:CG2	2.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLY:HA3	1:D:70:LEU:HD23	1.58	0.83
1:D:238:TRP:O	1:D:242:THR:CG2	2.26	0.83
1:D:238:TRP:O	1:D:242:THR:HG23	1.79	0.81
1:B:87:ALA:O	1:B:88:THR:HB	1.78	0.81
1:B:134:GLU:O	1:B:135:ALA:HB2	1.83	0.79
1:B:38:ASN:HA	1:B:52:ASN:HD21	1.48	0.78
1:A:170:ARG:HG2	1:A:170:ARG:NH1	1.98	0.76
1:C:137:ILE:O	1:C:137:ILE:CG1	2.35	0.74
1:B:170:ARG:CG	1:B:170:ARG:HH11	1.94	0.74
1:B:27:GLU:HB2	1:B:280:ILE:HG21	1.69	0.74
1:B:270:LEU:HD23	1:B:276:THR:HA	1.71	0.71
1:D:222:LEU:HD22	1:D:223:PRO:HD2	1.74	0.70
1:B:38:ASN:HA	1:B:52:ASN:ND2	2.06	0.70
1:A:2:LEU:HD12	1:A:25:THR:HG22	1.74	0.69
1:B:204:MET:HA	1:B:208:LEU:O	1.92	0.69
1:C:170:ARG:CG	1:C:170:ARG:HH11	2.05	0.68
1:A:126:LEU:HD12	1:A:159:ILE:CD1	2.22	0.68
1:B:88:THR:HG21	1:D:190:ARG:HH22	1.59	0.68
1:B:134:GLU:O	1:B:135:ALA:HB3	1.91	0.68
1:A:24:PHE:CB	1:A:280:ILE:CD1	2.69	0.67
1:D:332:ASN:O	1:D:333:GLN:CD	2.33	0.67
1:D:332:ASN:O	1:D:333:GLN:HB2	1.94	0.67
1:C:170:ARG:HG2	1:C:170:ARG:HH11	1.60	0.67
1:B:27:GLU:CB	1:B:280:ILE:HG21	2.25	0.66
1:D:31:LYS:HB2	1:D:320:PHE:O	1.95	0.66
1:C:137:ILE:O	1:C:139:LEU:N	2.28	0.66
1:D:332:ASN:O	1:D:333:GLN:CB	2.44	0.64
1:C:136:ASN:C	1:C:138:ILE:H	2.00	0.64
1:C:43:LEU:HD12	1:C:103:ILE:HG13	1.79	0.63
1:A:208:LEU:HD13	1:A:210:LEU:HD21	1.80	0.63
1:C:32:VAL:HG13	1:C:320:PHE:HB2	1.79	0.63
1:B:256:PHE:CD2	1:B:295:LYS:HE2	2.33	0.63
1:A:57:PHE:HE1	1:A:70:LEU:HD13	1.65	0.62
1:D:242:THR:HG21	1:D:258:ILE:CG1	2.29	0.62
1:C:137:ILE:HG12	1:C:139:LEU:CB	2.29	0.61
1:C:137:ILE:C	1:C:139:LEU:N	2.52	0.61
1:B:136:ASN:HD22	1:B:136:ASN:N	1.98	0.61
1:D:238:TRP:O	1:D:242:THR:HG22	1.98	0.61
1:C:137:ILE:O	1:C:138:ILE:C	2.37	0.61
1:B:4:SER:HB2	1:B:21:THR:O	2.01	0.61
1:A:53:ASN:HA	1:A:115:ASN:HD21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:SER:HB3	1:D:21:THR:O	2.01	0.60
1:B:170:ARG:CG	1:B:170:ARG:NH1	2.58	0.60
1:B:87:ALA:O	1:B:88:THR:CB	2.50	0.60
1:D:1:MET:HE1	1:D:4:SER:OG	2.01	0.60
1:C:42:ARG:NH1	1:C:48:ASN:ND2	2.50	0.60
1:C:149:PHE:HE2	1:C:159:ILE:HD13	1.67	0.60
1:C:208:LEU:HD13	1:C:210:LEU:HD13	1.84	0.59
1:C:149:PHE:CE2	1:C:159:ILE:HD13	2.38	0.58
1:B:102:GLY:HA3	1:B:132:LEU:HD22	1.84	0.58
1:B:301:ARG:HB2	1:C:301:ARG:HG3	1.85	0.58
1:D:138:ILE:HD13	2:D:2015:HOH:O	2.03	0.58
1:D:57:PHE:HE1	1:D:70:LEU:HD13	1.68	0.58
1:B:213:PHE:CE1	1:C:180:PRO:HG3	2.38	0.58
1:C:170:ARG:HG2	1:C:170:ARG:NH1	2.18	0.58
1:D:137:ILE:N	1:D:137:ILE:HD13	2.19	0.58
1:C:42:ARG:HG2	1:C:67:SER:OG	2.04	0.57
1:C:39:TYR:CE1	1:C:317:LEU:HD13	2.39	0.57
1:C:137:ILE:HG12	1:C:139:LEU:HB2	1.86	0.57
1:A:42:ARG:NH2	1:A:45:GLU:O	2.39	0.56
1:B:222:LEU:HD22	1:B:223:PRO:HD2	1.87	0.56
1:D:76:GLU:HG3	1:D:77:LYS:HD3	1.86	0.56
1:C:42:ARG:HH11	1:C:48:ASN:ND2	2.04	0.56
1:A:126:LEU:HD12	1:A:159:ILE:HD13	1.87	0.56
1:B:238:TRP:O	1:B:242:THR:HG22	2.05	0.55
1:D:173:ILE:HD13	1:D:189:LEU:HD11	1.87	0.55
1:A:180:PRO:HG3	1:D:213:PHE:CE1	2.41	0.55
1:B:136:ASN:ND2	1:B:136:ASN:N	2.53	0.55
1:C:37:ARG:NH1	1:C:76:GLU:OE1	2.39	0.55
1:A:119:VAL:HG13	1:A:157:ILE:HG21	1.88	0.55
1:C:137:ILE:CG1	1:C:139:LEU:HB2	2.37	0.55
1:C:9:ILE:HG23	1:C:255:LEU:HD21	1.87	0.54
1:D:148:THR:HB	1:D:176:MET:CE	2.38	0.54
1:C:136:ASN:C	1:C:138:ILE:N	2.60	0.54
1:C:29:ASP:OD1	1:C:29:ASP:N	2.28	0.54
1:A:184:TRP:CD1	1:C:184:TRP:CD1	2.95	0.54
1:B:126:LEU:CD2	1:B:159:ILE:HG21	2.38	0.53
1:D:238:TRP:HA	1:D:238:TRP:CE3	2.43	0.53
1:D:95:GLU:CA	1:D:95:GLU:OE1	2.52	0.53
1:A:170:ARG:CG	1:A:170:ARG:HH11	2.14	0.53
1:A:11:THR:OG1	1:A:13:ASP:HB3	2.09	0.52
1:C:13:ASP:O	1:C:14:ASP:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLY:C	1:A:4:SER:OG	2.43	0.52
1:B:332:ASN:O	1:B:334:VAL:HG23	2.10	0.52
1:A:4:SER:HB3	1:A:21:THR:O	2.09	0.52
1:C:83:MET:C	1:C:84:LEU:HD12	2.30	0.52
1:B:300:SER:OG	1:C:300:SER:O	2.28	0.52
1:B:84:LEU:HD13	1:B:176:MET:CE	2.41	0.51
1:B:330:GLN:HB3	1:B:334:VAL:HG23	1.92	0.51
1:D:102:GLY:HA3	1:D:132:LEU:HD22	1.92	0.51
1:A:11:THR:C	1:A:13:ASP:H	2.12	0.51
1:D:126:LEU:HD22	1:D:159:ILE:HG21	1.93	0.51
1:B:27:GLU:CB	1:B:280:ILE:CG2	2.88	0.51
1:C:57:PHE:HB3	1:C:75:ASN:HA	1.93	0.50
1:A:20:ARG:HD2	1:A:72:ASP:OD2	2.11	0.50
1:C:291:ASN:HD22	1:C:306:SER:HA	1.76	0.50
1:A:146:HIS:HB2	1:A:160:GLU:HG2	1.93	0.50
1:A:1:MET:CG	2:A:2002:HOH:O	2.60	0.50
1:C:193:ILE:HB	1:D:203:ILE:HG12	1.94	0.50
1:D:238:TRP:HA	1:D:238:TRP:HE3	1.77	0.49
1:C:170:ARG:HH11	1:C:170:ARG:CB	2.25	0.49
1:B:38:ASN:CA	1:B:52:ASN:HD21	2.20	0.49
1:D:3:GLY:HA3	2:D:2002:HOH:O	2.13	0.49
1:D:222:LEU:HD11	1:D:234:ARG:HG3	1.93	0.49
1:C:240:LYS:HD3	1:C:241:TYR:CZ	2.47	0.48
1:C:137:ILE:HG12	1:C:139:LEU:HB3	1.94	0.48
1:C:31:LYS:HB2	1:C:320:PHE:O	2.13	0.48
1:B:27:GLU:HB2	1:B:280:ILE:CG2	2.40	0.48
1:A:109:ILE:HG22	1:A:113:LEU:HD22	1.96	0.48
1:D:119:VAL:HA	1:D:122:VAL:HG13	1.96	0.48
1:D:227:THR:HB	1:D:228:PRO:CD	2.44	0.48
1:B:22:MET:O	1:B:280:ILE:HG13	2.14	0.47
1:B:83:MET:C	1:B:84:LEU:HD12	2.34	0.47
1:B:184:TRP:CD1	1:D:184:TRP:CD1	3.01	0.47
1:B:238:TRP:HA	1:B:238:TRP:CE3	2.49	0.47
1:B:126:LEU:HD21	1:B:159:ILE:HG21	1.95	0.47
1:D:1:MET:HE2	1:D:1:MET:HB3	1.45	0.47
1:B:88:THR:HG21	1:D:190:ARG:NH2	2.28	0.47
1:D:1:MET:CE	1:D:4:SER:OG	2.62	0.47
1:A:2:LEU:HD12	1:A:25:THR:CG2	2.41	0.47
1:B:301:ARG:HG2	2:B:2067:HOH:O	2.14	0.47
1:D:26:MET:O	1:D:28:PRO:HD3	2.13	0.47
1:D:242:THR:HG21	1:D:258:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD12	1:A:159:ILE:HD12	1.97	0.47
1:C:146:HIS:HB2	1:C:160:GLU:HG2	1.97	0.47
1:C:211:THR:OG1	1:C:212:PRO:HD2	2.15	0.47
1:C:43:LEU:HD13	1:C:111:GLN:NE2	2.29	0.47
1:A:57:PHE:CE1	1:A:70:LEU:HD13	2.47	0.46
1:B:291:ASN:HD22	1:B:306:SER:HA	1.80	0.46
1:A:24:PHE:CE2	1:A:28:PRO:HD3	2.49	0.46
1:C:211:THR:O	1:D:190:ARG:HB3	2.15	0.46
1:D:180:PRO:HD2	1:D:185:HIS:NE2	2.29	0.46
1:A:85:TYR:CZ	1:A:144:PRO:HD2	2.50	0.46
1:C:150:THR:HA	1:C:155:GLU:O	2.15	0.46
1:C:137:ILE:C	1:C:139:LEU:H	2.15	0.46
1:C:12:THR:OG1	1:C:246:LYS:HA	2.15	0.46
1:C:135:ALA:O	1:C:136:ASN:HB2	2.16	0.46
1:C:208:LEU:HD13	1:C:210:LEU:CD1	2.46	0.46
1:B:27:GLU:HB3	1:B:280:ILE:CG2	2.46	0.46
1:D:9:ILE:HG12	1:D:255:LEU:HD21	1.98	0.46
1:B:4:SER:CB	1:B:21:THR:O	2.63	0.46
1:A:1:MET:HB2	1:A:1:MET:HE2	1.77	0.46
1:B:178:ASN:HB2	1:B:228:PRO:HB3	1.98	0.46
1:D:178:ASN:HB2	1:D:228:PRO:HB3	1.98	0.45
1:A:190:ARG:HB3	1:B:211:THR:O	2.17	0.45
1:D:231:ARG:HG2	1:D:262:VAL:HB	1.96	0.45
1:D:43:LEU:HD12	1:D:103:ILE:HG13	1.97	0.45
1:B:238:TRP:HE3	1:B:238:TRP:HA	1.82	0.45
1:B:334:VAL:HG12	1:B:334:VAL:O	2.17	0.45
1:D:180:PRO:HD2	1:D:185:HIS:CE1	2.52	0.45
1:D:106:VAL:HG13	1:D:106:VAL:O	2.16	0.45
1:D:196:THR:HB	1:D:197:PRO:HD2	1.98	0.45
1:B:146:HIS:HB2	1:B:160:GLU:HG2	1.99	0.44
1:A:204:MET:HG2	1:A:209:ASP:OD1	2.17	0.44
1:D:1:MET:HE1	1:D:4:SER:HG	1.82	0.44
1:C:33:ILE:O	1:C:58:VAL:HA	2.17	0.44
1:D:79:LEU:HD13	1:D:113:LEU:HD12	2.00	0.44
1:A:42:ARG:HG2	1:A:50:VAL:HG22	2.00	0.44
1:C:84:LEU:O	1:C:146:HIS:HD2	2.00	0.44
1:B:27:GLU:OE1	1:B:324:ARG:HD3	2.17	0.44
1:B:208:LEU:HA	1:B:208:LEU:HD23	1.78	0.44
1:D:231:ARG:HG2	1:D:262:VAL:CG1	2.47	0.44
1:C:25:THR:HA	1:C:276:THR:O	2.16	0.43
1:A:24:PHE:CD2	1:A:26:MET:O	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:CG2	1:A:131:LEU:HD12	2.48	0.43
1:C:211:THR:OG1	1:C:212:PRO:CD	2.66	0.43
1:D:242:THR:HG21	1:D:258:ILE:HD11	2.01	0.43
1:D:227:THR:HB	1:D:228:PRO:HD2	2.00	0.43
1:A:11:THR:OG1	1:A:13:ASP:CB	2.66	0.43
1:B:268:VAL:HG23	1:B:269:VAL:HG23	2.00	0.43
1:D:146:HIS:HB2	1:D:160:GLU:HG2	2.00	0.43
1:D:57:PHE:CD2	1:D:57:PHE:N	2.87	0.43
1:C:146:HIS:CB	1:C:160:GLU:HG2	2.48	0.43
1:B:2:LEU:HD12	1:B:25:THR:HG22	2.00	0.43
1:A:298:ASP:OD2	1:A:324:ARG:HG2	2.19	0.43
1:D:196:THR:HB	1:D:197:PRO:CD	2.48	0.43
1:C:105:PRO:HG2	1:C:142:ALA:HB1	2.01	0.43
1:D:293:TYR:HA	1:D:303:SER:O	2.19	0.43
1:A:146:HIS:CB	1:A:160:GLU:HG2	2.49	0.42
1:D:43:LEU:HA	1:D:43:LEU:HD12	1.62	0.42
1:D:280:ILE:CG2	1:D:281:TYR:N	2.82	0.42
1:B:85:TYR:CE2	1:B:87:ALA:HB2	2.55	0.42
1:B:116:CYS:SG	1:B:125:LYS:HG2	2.58	0.42
1:D:222:LEU:CD1	1:D:234:ARG:HG3	2.50	0.42
1:C:289:SER:O	1:C:290:LYS:HB2	2.19	0.42
1:C:18:PHE:O	1:C:284:ALA:HA	2.19	0.42
1:C:1:MET:HG2	1:C:22:MET:SD	2.60	0.42
1:A:160:GLU:HA	1:A:161:PRO:HD3	1.92	0.42
1:B:317:LEU:HA	1:B:317:LEU:HD12	1.83	0.42
1:D:172:THR:HB	1:D:182:TYR:CZ	2.54	0.42
1:D:61:GLY:HA3	1:D:69:VAL:O	2.20	0.42
1:A:39:TYR:CE1	1:A:317:LEU:HD13	2.55	0.42
1:B:88:THR:HG22	1:B:88:THR:O	2.19	0.41
1:B:205:MET:N	1:B:208:LEU:O	2.50	0.41
1:D:170:ARG:NH1	1:D:170:ARG:HB2	2.35	0.41
1:B:150:THR:HA	1:B:155:GLU:O	2.20	0.41
1:C:222:LEU:HD12	1:C:238:TRP:CZ2	2.55	0.41
1:D:222:LEU:CD2	1:D:223:PRO:HD2	2.47	0.41
1:D:170:ARG:HH11	1:D:170:ARG:HB2	1.84	0.41
1:A:323:ASP:C	1:A:323:ASP:OD1	2.59	0.41
1:B:56:ALA:CB	1:B:312:LEU:HD22	2.50	0.41
1:D:278:TYR:CZ	1:D:280:ILE:HD12	2.55	0.41
1:B:43:LEU:HA	1:B:43:LEU:HD12	1.96	0.41
1:D:59:GLY:CA	1:D:70:LEU:HD23	2.41	0.41
1:D:112:VAL:HG11	1:D:149:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:HE2	2:A:2009:HOH:O	2.20	0.41
1:A:188:ASN:HD22	1:C:184:TRP:HZ2	1.69	0.41
1:B:103:ILE:HD11	1:B:111:GLN:HG3	2.03	0.41
1:C:240:LYS:NZ	1:D:204:MET:O	2.49	0.41
1:B:119:VAL:HG21	1:B:155:GLU:HG2	2.01	0.41
1:A:76:GLU:O	1:A:290:LYS:HE2	2.21	0.41
1:D:238:TRP:CE3	1:D:238:TRP:CA	3.03	0.41
1:B:26:MET:O	1:B:27:GLU:HG2	2.20	0.41
1:C:178:ASN:HB2	1:C:228:PRO:HB3	2.03	0.41
1:D:45:GLU:OE2	1:D:66:THR:OG1	2.38	0.41
1:A:40:GLY:O	1:A:41:ILE:HD13	2.21	0.41
1:D:125:LYS:HD3	1:D:125:LYS:HA	1.83	0.40
1:D:259:LEU:HD23	1:D:259:LEU:HA	1.91	0.40
1:B:34:ILE:HD13	1:B:310:GLU:HG3	2.02	0.40
1:A:24:PHE:HE2	1:A:28:PRO:HD3	1.85	0.40
1:D:15:LYS:HD2	1:D:248:GLU:HB2	2.03	0.40
1:B:84:LEU:HD13	1:B:176:MET:HE2	2.03	0.40
1:A:141:PHE:O	1:A:143:PRO:HD3	2.22	0.40
1:D:122:VAL:HG22	1:D:157:ILE:HD11	2.03	0.40
1:A:141:PHE:CD2	1:A:141:PHE:N	2.89	0.40
1:A:303:SER:HB3	1:D:331:LEU:HD22	2.03	0.40
1:B:76:GLU:O	1:B:290:LYS:HE2	2.21	0.40
1:C:11:THR:HG1	1:C:15:LYS:H	1.68	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	332/338 (98%)	314 (95%)	16 (5%)	2 (1%)	30 50
1	B	332/338 (98%)	310 (93%)	16 (5%)	6 (2%)	11 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	331/338 (98%)	306 (92%)	22 (7%)	3 (1%)	21 37
1	D	331/338 (98%)	316 (96%)	15 (4%)	0	100 100
All	All	1326/1352 (98%)	1246 (94%)	69 (5%)	11 (1%)	24 41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	LEU
1	B	135	ALA
1	B	138	ILE
1	B	209	ASP
1	C	136	ASN
1	C	137	ILE
1	A	2	LEU
1	A	4	SER
1	C	138	ILE
1	B	27	GLU
1	B	28	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	290/294 (99%)	257 (89%)	33 (11%)	7 13
1	B	290/294 (99%)	250 (86%)	40 (14%)	4 8
1	C	289/294 (98%)	246 (85%)	43 (15%)	4 6
1	D	289/294 (98%)	247 (86%)	42 (14%)	4 7
All	All	1158/1176 (98%)	1000 (86%)	158 (14%)	5 8

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	SER
1	A	20	ARG
1	A	25	THR
1	A	26	MET
1	A	27	GLU
1	A	31	LYS
1	A	32	VAL
1	A	43	LEU
1	A	44	LEU
1	A	70	LEU
1	A	85	TYR
1	A	106	VAL
1	A	113	LEU
1	A	125	LYS
1	A	146	HIS
1	A	170	ARG
1	A	198	ASN
1	A	208	LEU
1	A	215	GLN
1	A	222	LEU
1	A	238	TRP
1	A	244	LYS
1	A	246	LYS
1	A	272	ASN
1	A	276	THR
1	A	285	MET
1	A	290	LYS
1	A	306	SER
1	A	317	LEU
1	A	328	ILE
1	A	331	LEU
1	B	1	MET
1	B	2	LEU
1	B	20	ARG
1	B	25	THR
1	B	26	MET
1	B	31	LYS
1	B	37	ARG
1	B	43	LEU
1	B	44	LEU
1	B	48	ASN

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Mol	Chain	Res	Type
1	B	85	TYR
1	B	101	ARG
1	B	113	LEU
1	B	125	LYS
1	B	132	LEU
1	B	133	ASN
1	B	134	GLU
1	B	136	ASN
1	B	137	ILE
1	B	145	LEU
1	B	146	HIS
1	B	170	ARG
1	B	204	MET
1	B	222	LEU
1	B	233	LEU
1	B	238	TRP
1	B	242	THR
1	B	244	LYS
1	B	260	SER
1	B	276	THR
1	B	280	ILE
1	B	290	LYS
1	B	299	ASN
1	B	300	SER
1	B	315	GLN
1	B	317	LEU
1	B	324	ARG
1	B	330	GLN
1	B	331	LEU
1	B	333	GLN
1	C	1	MET
1	C	2	LEU
1	C	13	ASP
1	C	20	ARG
1	C	27	GLU
1	C	29	ASP
1	C	31	LYS
1	C	32	VAL
1	C	34	ILE
1	C	42	ARG
1	C	43	LEU
1	C	44	LEU

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Mol	Chain	Res	Type
1	C	46	LYS
1	C	48	ASN
1	C	85	TYR
1	C	98	LYS
1	C	106	VAL
1	C	113	LEU
1	C	120	ASP
1	C	126	LEU
1	C	136	ASN
1	C	137	ILE
1	C	139	LEU
1	C	146	HIS
1	C	153	SER
1	C	170	ARG
1	C	208	LEU
1	C	209	ASP
1	C	210	LEU
1	C	222	LEU
1	C	238	TRP
1	C	244	LYS
1	C	246	LYS
1	C	260	SER
1	C	266	LYS
1	C	273	GLU
1	C	275	LYS
1	C	276	THR
1	C	314	SER
1	C	317	LEU
1	C	319	THR
1	C	325	LYS
1	C	333	GLN
1	D	1	MET
1	D	4	SER
1	D	20	ARG
1	D	25	THR
1	D	26	MET
1	D	27	GLU
1	D	31	LYS
1	D	43	LEU
1	D	72	ASP
1	D	79	LEU
1	D	85	TYR

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Mol	Chain	Res	Type
1	D	95	GLU
1	D	97	LYS
1	D	106	VAL
1	D	113	LEU
1	D	120	ASP
1	D	125	LYS
1	D	126	LEU
1	D	132	LEU
1	D	137	ILE
1	D	138	ILE
1	D	139	LEU
1	D	145	LEU
1	D	146	HIS
1	D	163	LYS
1	D	170	ARG
1	D	171	LYS
1	D	222	LEU
1	D	238	TRP
1	D	242	THR
1	D	243	GLU
1	D	268	VAL
1	D	276	THR
1	D	280	ILE
1	D	285	MET
1	D	290	LYS
1	D	312	LEU
1	D	315	GLN
1	D	317	LEU
1	D	321	GLU
1	D	331	LEU
1	D	333	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	52	ASN
1	A	115	ASN
1	A	133	ASN
1	A	188	ASN
1	A	315	GLN
1	B	38	ASN

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Mol	Chain	Res	Type
1	B	52	ASN
1	B	133	ASN
1	B	136	ASN
1	B	186	GLN
1	B	188	ASN
1	B	254	ASN
1	B	291	ASN
1	B	299	ASN
1	B	333	GLN
1	C	38	ASN
1	C	48	ASN
1	C	52	ASN
1	C	186	GLN
1	C	188	ASN
1	C	215	GLN
1	C	254	ASN
1	C	291	ASN
1	C	315	GLN
1	D	38	ASN
1	D	52	ASN
1	D	188	ASN
1	D	215	GLN
1	D	291	ASN
1	D	315	GLN

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.