Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 10:51 pm GMT

PDB ID	:	2XWG
Title	:	Crystal structure of sortase C-1 from Actinomyces oris (formerly Actinomyces naeslundii)
Authors	:	Persson, K.
Deposited on	:	2010-11-02
Resolution	:	2.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

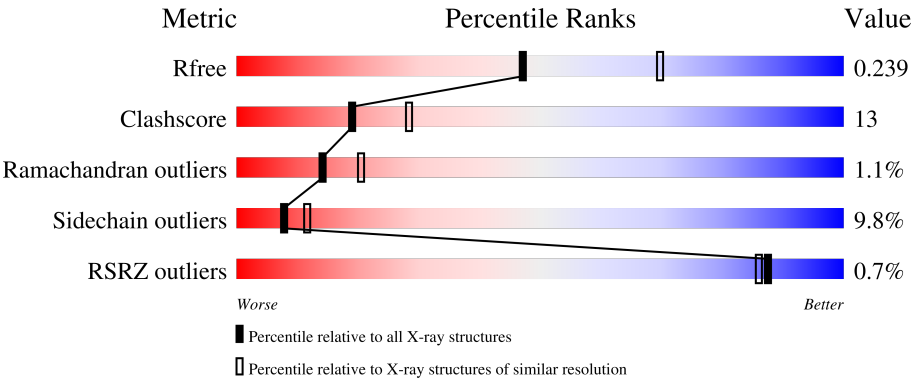
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 >=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 <=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	235	59% 14% · 23%
1	B	235	63% 12% · 21%
1	C	235	57% 14% · 25%
1	D	235	% 56% 18% · 22%
1	E	235	% 52% 18% 5% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7181 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 SORTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1399	881	238	275	5			
1	B	185	Total	C	N	O	S	0	0	0
			1423	895	242	281	5			
1	C	176	Total	C	N	O	S	0	0	0
			1357	857	229	266	5			
1	D	184	Total	C	N	O	S	0	0	0
			1414	889	241	279	5			
1	E	177	Total	C	N	O	S	0	0	0
			1364	861	230	268	5			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	expression tag	UNP Q0Z952
A	55	LYS	-	expression tag	UNP Q0Z952
A	56	HIS	-	expression tag	UNP Q0Z952
A	57	HIS	-	expression tag	UNP Q0Z952
A	58	HIS	-	expression tag	UNP Q0Z952
A	59	HIS	-	expression tag	UNP Q0Z952
A	60	HIS	-	expression tag	UNP Q0Z952
A	61	HIS	-	expression tag	UNP Q0Z952
A	62	PRO	-	expression tag	UNP Q0Z952
A	63	MET	-	expression tag	UNP Q0Z952
A	64	SER	-	expression tag	UNP Q0Z952
A	65	ASP	-	expression tag	UNP Q0Z952
A	66	TYR	-	expression tag	UNP Q0Z952
A	67	ASP	-	expression tag	UNP Q0Z952
A	68	ILE	-	expression tag	UNP Q0Z952
A	69	PRO	-	expression tag	UNP Q0Z952
A	70	THR	-	expression tag	UNP Q0Z952
A	71	THR	-	expression tag	UNP Q0Z952
A	72	GLU	-	expression tag	UNP Q0Z952

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Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ASN	-	expression tag	UNP Q0Z952
A	74	LEU	-	expression tag	UNP Q0Z952
A	75	TYR	-	expression tag	UNP Q0Z952
A	76	PHE	-	expression tag	UNP Q0Z952
A	77	GLN	-	expression tag	UNP Q0Z952
B	54	MET	-	expression tag	UNP Q0Z952
B	55	LYS	-	expression tag	UNP Q0Z952
B	56	HIS	-	expression tag	UNP Q0Z952
B	57	HIS	-	expression tag	UNP Q0Z952
B	58	HIS	-	expression tag	UNP Q0Z952
B	59	HIS	-	expression tag	UNP Q0Z952
B	60	HIS	-	expression tag	UNP Q0Z952
B	61	HIS	-	expression tag	UNP Q0Z952
B	62	PRO	-	expression tag	UNP Q0Z952
B	63	MET	-	expression tag	UNP Q0Z952
B	64	SER	-	expression tag	UNP Q0Z952
B	65	ASP	-	expression tag	UNP Q0Z952
B	66	TYR	-	expression tag	UNP Q0Z952
B	67	ASP	-	expression tag	UNP Q0Z952
B	68	ILE	-	expression tag	UNP Q0Z952
B	69	PRO	-	expression tag	UNP Q0Z952
B	70	THR	-	expression tag	UNP Q0Z952
B	71	THR	-	expression tag	UNP Q0Z952
B	72	GLU	-	expression tag	UNP Q0Z952
B	73	ASN	-	expression tag	UNP Q0Z952
B	74	LEU	-	expression tag	UNP Q0Z952
B	75	TYR	-	expression tag	UNP Q0Z952
B	76	PHE	-	expression tag	UNP Q0Z952
B	77	GLN	-	expression tag	UNP Q0Z952
C	54	MET	-	expression tag	UNP Q0Z952
C	55	LYS	-	expression tag	UNP Q0Z952
C	56	HIS	-	expression tag	UNP Q0Z952
C	57	HIS	-	expression tag	UNP Q0Z952
C	58	HIS	-	expression tag	UNP Q0Z952
C	59	HIS	-	expression tag	UNP Q0Z952
C	60	HIS	-	expression tag	UNP Q0Z952
C	61	HIS	-	expression tag	UNP Q0Z952
C	62	PRO	-	expression tag	UNP Q0Z952
C	63	MET	-	expression tag	UNP Q0Z952
C	64	SER	-	expression tag	UNP Q0Z952
C	65	ASP	-	expression tag	UNP Q0Z952
C	66	TYR	-	expression tag	UNP Q0Z952

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Chain	Residue	Modelled	Actual	Comment	Reference
C	67	ASP	-	expression tag	UNP Q0Z952
C	68	ILE	-	expression tag	UNP Q0Z952
C	69	PRO	-	expression tag	UNP Q0Z952
C	70	THR	-	expression tag	UNP Q0Z952
C	71	THR	-	expression tag	UNP Q0Z952
C	72	GLU	-	expression tag	UNP Q0Z952
C	73	ASN	-	expression tag	UNP Q0Z952
C	74	LEU	-	expression tag	UNP Q0Z952
C	75	TYR	-	expression tag	UNP Q0Z952
C	76	PHE	-	expression tag	UNP Q0Z952
C	77	GLN	-	expression tag	UNP Q0Z952
D	54	MET	-	expression tag	UNP Q0Z952
D	55	LYS	-	expression tag	UNP Q0Z952
D	56	HIS	-	expression tag	UNP Q0Z952
D	57	HIS	-	expression tag	UNP Q0Z952
D	58	HIS	-	expression tag	UNP Q0Z952
D	59	HIS	-	expression tag	UNP Q0Z952
D	60	HIS	-	expression tag	UNP Q0Z952
D	61	HIS	-	expression tag	UNP Q0Z952
D	62	PRO	-	expression tag	UNP Q0Z952
D	63	MET	-	expression tag	UNP Q0Z952
D	64	SER	-	expression tag	UNP Q0Z952
D	65	ASP	-	expression tag	UNP Q0Z952
D	66	TYR	-	expression tag	UNP Q0Z952
D	67	ASP	-	expression tag	UNP Q0Z952
D	68	ILE	-	expression tag	UNP Q0Z952
D	69	PRO	-	expression tag	UNP Q0Z952
D	70	THR	-	expression tag	UNP Q0Z952
D	71	THR	-	expression tag	UNP Q0Z952
D	72	GLU	-	expression tag	UNP Q0Z952
D	73	ASN	-	expression tag	UNP Q0Z952
D	74	LEU	-	expression tag	UNP Q0Z952
D	75	TYR	-	expression tag	UNP Q0Z952
D	76	PHE	-	expression tag	UNP Q0Z952
D	77	GLN	-	expression tag	UNP Q0Z952
E	54	MET	-	expression tag	UNP Q0Z952
E	55	LYS	-	expression tag	UNP Q0Z952
E	56	HIS	-	expression tag	UNP Q0Z952
E	57	HIS	-	expression tag	UNP Q0Z952
E	58	HIS	-	expression tag	UNP Q0Z952
E	59	HIS	-	expression tag	UNP Q0Z952
E	60	HIS	-	expression tag	UNP Q0Z952

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Chain	Residue	Modelled	Actual	Comment	Reference
E	61	HIS	-	expression tag	UNP Q0Z952
E	62	PRO	-	expression tag	UNP Q0Z952
E	63	MET	-	expression tag	UNP Q0Z952
E	64	SER	-	expression tag	UNP Q0Z952
E	65	ASP	-	expression tag	UNP Q0Z952
E	66	TYR	-	expression tag	UNP Q0Z952
E	67	ASP	-	expression tag	UNP Q0Z952
E	68	ILE	-	expression tag	UNP Q0Z952
E	69	PRO	-	expression tag	UNP Q0Z952
E	70	THR	-	expression tag	UNP Q0Z952
E	71	THR	-	expression tag	UNP Q0Z952
E	72	GLU	-	expression tag	UNP Q0Z952
E	73	ASN	-	expression tag	UNP Q0Z952
E	74	LEU	-	expression tag	UNP Q0Z952
E	75	TYR	-	expression tag	UNP Q0Z952
E	76	PHE	-	expression tag	UNP Q0Z952
E	77	GLN	-	expression tag	UNP Q0Z952

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is water.

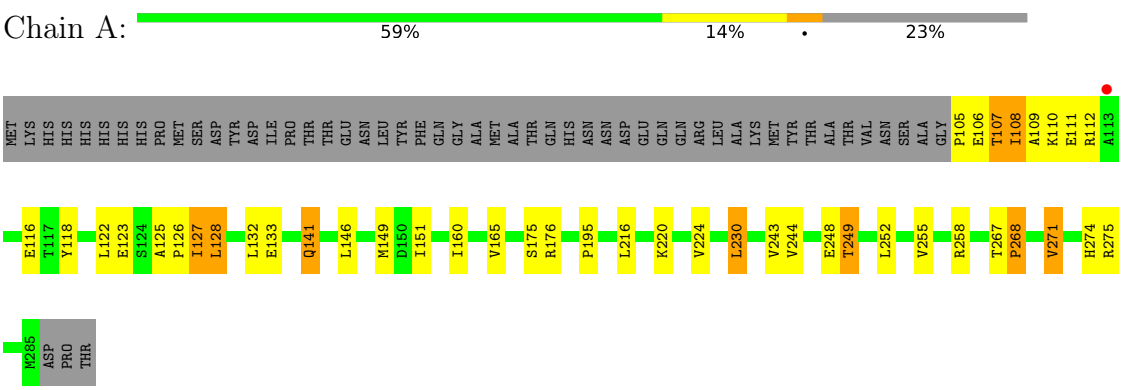
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	43	Total O 43 43	0	0
3	B	69	Total O 69 69	0	0
3	C	48	Total O 48 48	0	0
3	D	44	Total O 44 44	0	0
3	E	16	Total O 16 16	0	0

3 Residue-property plots (i)

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.

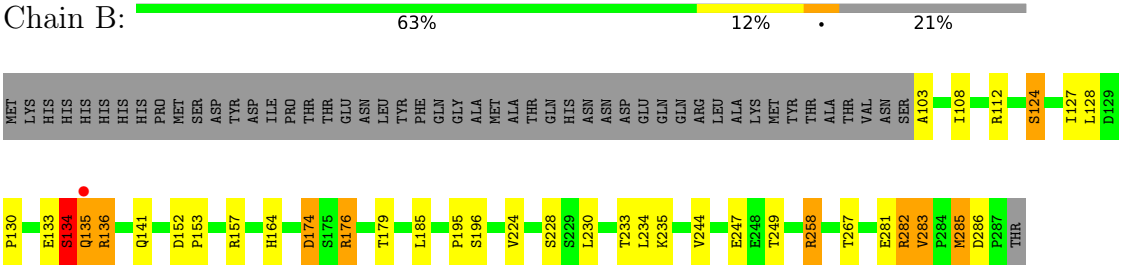
- Molecule 1: SORTASE

Chain A:



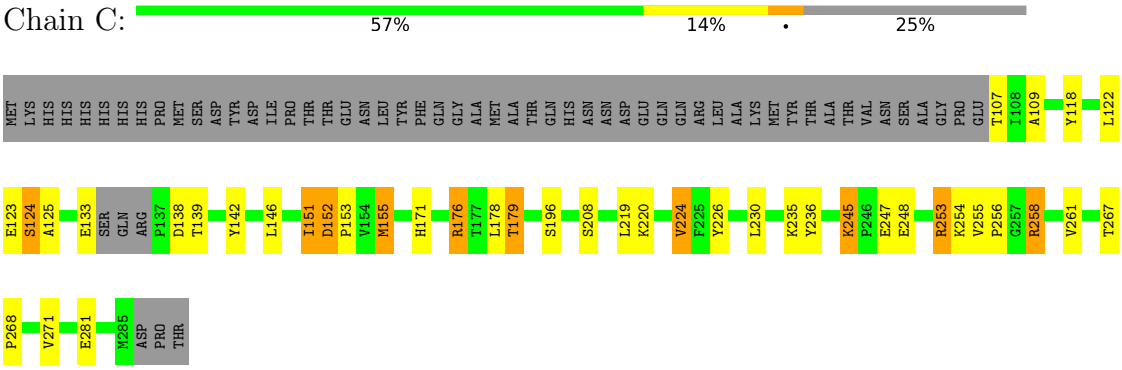
- Molecule 1: SORTASE

Chain B:



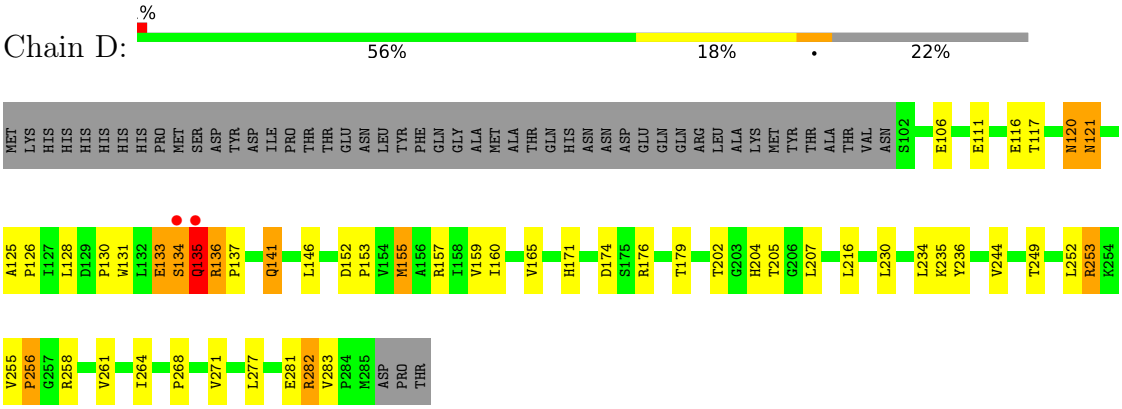
- Molecule 1: SORTASE

Chain C:



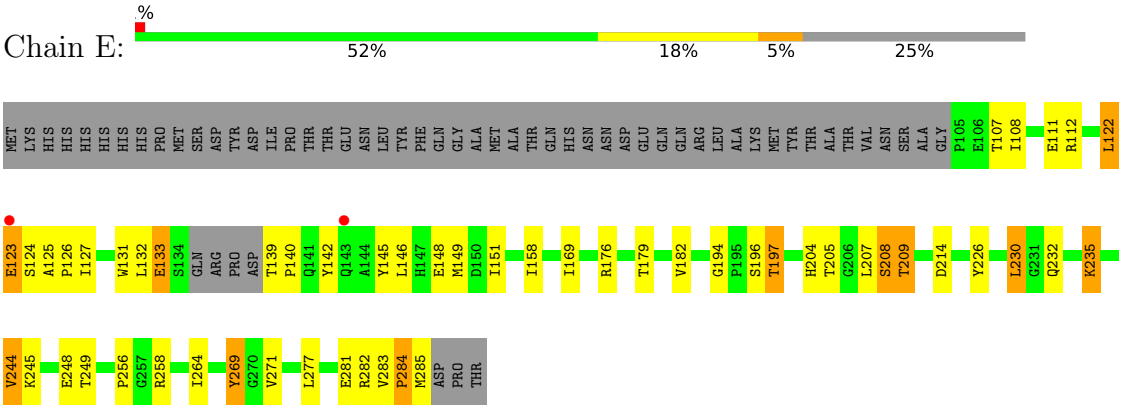
- Molecule 1: SORTASE

Chain D:



• Molecule 1: SORTASE

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.07Å 108.23Å 143.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 2.40 44.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.6 (43.67-2.40) 91.4 (44.57-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.205 , 0.244 0.202 , 0.239	Depositor DCC
R_{free} test set	3060 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7181	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.52	0/1431	0.65	0/1955
1	B	0.54	0/1456	0.74	0/1991
1	C	0.53	0/1387	0.69	0/1894
1	D	0.52	0/1446	0.74	1/1976 (0.1%)
1	E	0.46	0/1394	0.62	0/1903
All	All	0.51	0/7114	0.69	1/9719 (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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	120	ASN	N-CA-C	5.62	126.19	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	135	GLN	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	1399	0	1387	34	0
1	B	1423	0	1405	33	0
1	C	1357	0	1347	27	0
1	D	1414	0	1399	45	0
1	E	1364	0	1354	42	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	43	0	0	1	0
3	B	69	0	0	1	0
3	C	48	0	0	1	0
3	D	44	0	0	1	0
3	E	16	0	0	2	0
All	All	7181	0	6892	180	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 13.

All (180) 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:E:111:GLU:HG3	1:E:151:ILE:HD11	1.34	1.10
1:C:139:THR:HG23	1:C:142:TYR:H	1.17	1.09
1:E:122:LEU:HA	1:E:123:GLU:CB	1.86	1.05
1:E:122:LEU:HA	1:E:123:GLU:HB2	1.40	1.01
1:B:135:GLN:HB2	1:B:136:ARG:CB	1.97	0.94
1:D:268:PRO:HD2	1:D:271:VAL:HG22	1.59	0.84
1:E:235:LYS:HD2	1:E:283:VAL:HG23	1.60	0.81
1:B:135:GLN:HB2	1:B:136:ARG:HB3	1.59	0.81
1:C:139:THR:CG2	1:C:142:TYR:H	1.95	0.77
1:B:136:ARG:N	1:B:136:ARG:HD2	2.02	0.75
1:A:106:GLU:CG	1:A:109:ALA:HB2	2.15	0.75
1:D:253:ARG:HH11	1:D:253:ARG:HG2	1.51	0.74
1:D:128:LEU:HD13	1:D:133:GLU:HG3	1.70	0.74
1:D:253:ARG:HH11	1:D:253:ARG:CG	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:LEU:HA	1:E:123:GLU:HB3	1.70	0.73
1:E:258:ARG:HD3	1:E:281:GLU:OE2	1.88	0.73
1:C:152:ASP:OD1	1:C:153:PRO:HD2	1.89	0.72
1:E:207:LEU:CD1	1:E:209:THR:HG22	2.20	0.71
1:D:204:HIS:CD2	1:D:207:LEU:HD21	2.25	0.71
1:B:135:GLN:HB2	1:B:136:ARG:CG	2.21	0.71
1:B:133:GLU:O	1:B:135:GLN:HG2	1.89	0.71
1:B:135:GLN:CB	1:B:136:ARG:HG3	2.21	0.71
1:E:284:PRO:O	1:E:285:MET:HB2	1.91	0.70
1:E:226:TYR:CE1	1:E:235:LYS:HG3	2.28	0.69
1:A:106:GLU:HG2	1:A:109:ALA:HB2	1.72	0.69
1:B:135:GLN:HB2	1:B:136:ARG:HG3	1.72	0.69
1:A:195:PRO:HD2	3:A:2022:HOH:O	1.91	0.69
1:C:139:THR:HG22	1:C:142:TYR:HB2	1.73	0.69
1:A:111:GLU:HG3	1:A:151:ILE:HD11	1.74	0.69
1:E:207:LEU:HD11	1:E:209:THR:HG22	1.75	0.67
1:E:111:GLU:HG3	1:E:151:ILE:CD1	2.19	0.67
1:D:202:THR:HG22	1:D:264:ILE:CG2	2.25	0.66
1:D:133:GLU:O	1:D:134:SER:O	2.14	0.66
1:D:155:MET:HE1	1:D:171:HIS:CG	2.31	0.66
1:E:208:SER:HB3	3:E:2005:HOH:O	1.95	0.65
1:B:135:GLN:HG3	1:B:136:ARG:HG3	1.78	0.64
1:E:142:TYR:CE2	1:E:146:LEU:HD11	2.32	0.64
1:B:128:LEU:HD22	1:B:133:GLU:HG3	1.80	0.64
1:D:258:ARG:HD2	1:D:281:GLU:OE2	1.98	0.63
1:C:123:GLU:HG2	3:C:2004:HOH:O	1.99	0.62
1:C:255:VAL:HG12	1:C:258:ARG:HG3	1.82	0.62
1:D:236:TYR:CE2	1:D:261:VAL:HG23	2.35	0.62
1:E:244:VAL:HG13	1:E:248:GLU:HB3	1.81	0.61
1:D:253:ARG:HG2	1:D:253:ARG:NH1	2.15	0.61
1:A:127:ILE:HD12	1:A:252:LEU:HB2	1.82	0.61
1:D:157:ARG:HD3	3:D:2012:HOH:O	2.00	0.61
1:D:136:ARG:HH11	1:D:136:ARG:HG3	1.65	0.61
1:E:122:LEU:CA	1:E:123:GLU:CB	2.69	0.60
1:C:139:THR:HG23	1:C:142:TYR:N	2.02	0.60
1:E:151:ILE:N	1:E:151:ILE:HD13	2.15	0.60
1:E:207:LEU:HD13	1:E:209:THR:H	1.65	0.60
1:A:133:GLU:HA	1:A:133:GLU:OE1	2.02	0.59
1:E:194:GLY:O	1:E:197:THR:HB	2.02	0.59
1:B:195:PRO:O	1:B:196:SER:HB2	2.02	0.58
1:A:274:HIS:O	1:A:275:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ILE:HG13	1:E:277:LEU:CD2	2.33	0.58
1:A:125:ALA:HB1	1:A:126:PRO:CD	2.34	0.58
1:D:128:LEU:CD1	1:D:133:GLU:HG3	2.33	0.57
1:A:255:VAL:HG11	1:A:258:ARG:HD3	1.86	0.57
1:A:127:ILE:O	1:A:249:THR:HG21	2.05	0.57
1:B:103:ALA:N	3:B:2001:HOH:O	2.38	0.57
1:B:282:ARG:HG3	1:B:283:VAL:N	2.20	0.57
1:A:112:ARG:O	1:A:116:GLU:HG3	2.06	0.56
1:D:253:ARG:HH11	1:D:253:ARG:CB	2.18	0.56
1:D:120:ASN:CA	1:D:121:ASN:HB2	2.36	0.56
1:C:226:TYR:CE1	1:C:235:LYS:HD2	2.40	0.56
1:B:135:GLN:CG	1:B:136:ARG:HG3	2.35	0.55
1:B:258:ARG:HG2	1:B:281:GLU:OE2	2.06	0.55
1:A:141:GLN:NE2	1:A:141:GLN:H	2.04	0.55
1:A:128:LEU:HD12	1:A:132:LEU:HD22	1.89	0.55
1:E:139:THR:N	1:E:140:PRO:CD	2.70	0.55
1:D:155:MET:HE2	1:D:171:HIS:CE1	2.42	0.54
1:C:176:ARG:O	1:C:179:THR:HB	2.07	0.54
1:B:130:PRO:HG3	1:B:185:LEU:HD13	1.89	0.54
1:B:152:ASP:HB3	1:B:153:PRO:HD2	1.91	0.53
1:C:219:LEU:C	1:C:220:LYS:HD2	2.29	0.53
1:E:125:ALA:HB1	1:E:126:PRO:HD2	1.90	0.52
1:A:149:MET:HE3	1:A:230:LEU:HD22	1.92	0.52
1:B:133:GLU:HA	1:B:133:GLU:OE1	2.09	0.52
1:D:202:THR:HG22	1:D:264:ILE:HG22	1.92	0.52
1:A:255:VAL:CG1	1:A:258:ARG:HD3	2.40	0.52
1:D:120:ASN:HB2	1:D:121:ASN:HB2	1.92	0.51
1:E:127:ILE:HB	1:E:249:THR:HG21	1.91	0.51
1:A:106:GLU:HG3	1:A:109:ALA:H	1.75	0.51
1:B:133:GLU:O	1:B:134:SER:C	2.49	0.51
1:C:226:TYR:HE1	1:C:235:LYS:HD2	1.75	0.51
1:B:135:GLN:HB2	1:B:136:ARG:CA	2.40	0.51
1:B:258:ARG:HG2	1:B:258:ARG:HH11	1.75	0.51
1:A:106:GLU:CG	1:A:109:ALA:CB	2.87	0.51
1:D:155:MET:CE	1:D:171:HIS:CG	2.95	0.50
1:B:135:GLN:C	1:B:136:ARG:HD2	2.32	0.50
1:D:236:TYR:CZ	1:D:261:VAL:HG23	2.47	0.50
1:D:125:ALA:HB1	1:D:126:PRO:HD2	1.93	0.50
1:D:130:PRO:HG2	1:D:131:TRP:CE3	2.47	0.50
1:D:234:LEU:HD22	1:D:282:ARG:CZ	2.43	0.49
1:E:169:ILE:HA	1:E:182:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:SER:O	1:C:125:ALA:HB3	2.12	0.49
1:A:106:GLU:HG3	1:A:109:ALA:CB	2.43	0.49
1:D:135:GLN:HA	1:D:135:GLN:OE1	2.12	0.48
1:B:234:LEU:HD22	1:B:282:ARG:NH2	2.28	0.48
1:E:235:LYS:CD	1:E:283:VAL:HG23	2.39	0.48
1:D:160:ILE:HB	1:D:165:VAL:HB	1.95	0.48
1:D:155:MET:HE1	1:D:171:HIS:HA	1.96	0.48
1:E:142:TYR:O	1:E:145:TYR:HB3	2.13	0.48
1:E:148:GLU:O	1:E:149:MET:C	2.52	0.48
1:D:235:LYS:HD3	1:D:283:VAL:HG23	1.95	0.48
1:B:174:ASP:OD1	1:B:176:ARG:HB2	2.14	0.47
1:B:136:ARG:N	1:B:136:ARG:CD	2.66	0.47
1:D:136:ARG:HG3	1:D:136:ARG:NH1	2.29	0.47
1:C:224:VAL:HG21	1:C:235:LYS:HE3	1.96	0.47
1:D:152:ASP:OD2	1:D:153:PRO:HD2	2.14	0.47
1:D:255:VAL:O	1:D:255:VAL:HG12	2.15	0.47
1:C:245:LYS:HB2	1:C:248:GLU:OE2	2.13	0.47
1:C:267:THR:OG1	1:C:268:PRO:HA	2.14	0.47
1:D:135:GLN:NE2	1:D:174:ASP:HA	2.30	0.47
1:E:132:LEU:O	1:E:133:GLU:HB2	2.15	0.47
1:E:122:LEU:CA	1:E:123:GLU:HB3	2.42	0.47
1:C:118:TYR:CE2	1:C:122:LEU:HD13	2.50	0.47
1:C:253:ARG:CG	1:C:253:ARG:HH11	2.28	0.47
1:D:253:ARG:CG	1:D:253:ARG:NH1	2.69	0.46
1:A:111:GLU:HG3	1:A:151:ILE:CG1	2.45	0.46
1:B:235:LYS:HB2	1:B:285:MET:HG2	1.97	0.46
1:D:155:MET:HE1	1:D:171:HIS:CD2	2.49	0.46
1:B:157:ARG:HH11	1:B:157:ARG:HG3	1.80	0.46
1:D:176:ARG:HE	1:D:176:ARG:HB2	1.34	0.46
1:B:233:THR:HB	1:B:285:MET:HE3	1.98	0.46
1:E:176:ARG:O	1:E:179:THR:HB	2.16	0.46
1:A:111:GLU:HG3	1:A:151:ILE:CD1	2.42	0.45
1:D:255:VAL:HA	1:D:256:PRO:HD2	1.77	0.45
1:A:107:THR:HA	1:A:110:LYS:HE3	1.98	0.45
1:E:127:ILE:HB	1:E:249:THR:CG2	2.46	0.45
1:B:258:ARG:HG2	1:B:258:ARG:NH1	2.31	0.45
1:B:108:ILE:O	1:B:112:ARG:HG3	2.16	0.45
1:D:130:PRO:HG2	1:D:131:TRP:CZ3	2.52	0.45
1:A:244:VAL:HG13	1:A:248:GLU:HB2	1.98	0.45
1:E:149:MET:CE	1:E:230:LEU:HD22	2.47	0.45
1:C:151:ILE:O	1:C:151:ILE:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:PRO:HD2	1:A:271:VAL:HG13	1.99	0.44
1:E:131:TRP:HE1	1:E:204:HIS:CE1	2.35	0.44
1:D:152:ASP:CG	1:D:153:PRO:HD2	2.38	0.44
1:E:158:ILE:HG23	1:E:158:ILE:O	2.18	0.44
1:D:141:GLN:HE21	1:D:141:GLN:HB3	1.59	0.44
1:A:118:TYR:CE1	1:A:122:LEU:HD13	2.53	0.43
1:D:120:ASN:CB	1:D:121:ASN:HB2	2.48	0.43
1:C:236:TYR:CZ	1:C:261:VAL:HG23	2.54	0.43
1:E:269:TYR:HB2	3:E:2009:HOH:O	2.19	0.43
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.87	0.43
1:D:117:THR:O	1:D:121:ASN:CB	2.67	0.43
1:E:196:SER:OG	1:E:256:PRO:HA	2.18	0.43
1:D:111:GLU:HA	1:D:111:GLU:OE1	2.19	0.43
1:C:107:THR:HG22	1:C:109:ALA:N	2.33	0.42
1:E:149:MET:HE3	1:E:230:LEU:HD22	2.01	0.42
1:E:205:THR:HA	1:E:214:ASP:OD1	2.19	0.42
1:D:216:LEU:HD12	1:D:216:LEU:HA	1.81	0.42
1:A:125:ALA:HB1	1:A:126:PRO:HD2	2.01	0.42
1:A:105:PRO:HA	1:A:108:ILE:HG23	2.02	0.42
1:E:264:ILE:HG13	1:E:277:LEU:HD23	2.02	0.42
1:A:105:PRO:N	1:A:107:THR:CG2	2.83	0.41
1:C:253:ARG:CG	1:C:253:ARG:NH1	2.83	0.41
1:C:258:ARG:HD2	1:C:281:GLU:OE2	2.20	0.41
1:A:249:THR:O	1:A:249:THR:HG23	2.20	0.41
1:A:243:VAL:O	1:A:244:VAL:HG23	2.20	0.41
1:C:255:VAL:HA	1:C:256:PRO:HD3	1.84	0.41
1:B:234:LEU:HD22	1:B:282:ARG:CZ	2.49	0.41
1:B:233:THR:CG2	1:B:285:MET:HE3	2.51	0.41
1:D:252:LEU:HD21	1:D:277:LEU:HD13	2.03	0.41
1:C:178:LEU:HA	1:C:178:LEU:HD23	1.64	0.41
1:E:112:ARG:NH1	1:E:232:GLN:HB2	2.35	0.41
1:E:269:TYR:C	1:E:269:TYR:CD1	2.94	0.41
1:C:155:MET:CE	1:C:171:HIS:HA	2.51	0.41
1:C:220:LYS:HD2	1:C:220:LYS:N	2.36	0.41
1:A:106:GLU:HG3	1:A:109:ALA:N	2.36	0.41
1:A:175:SER:HA	1:B:164:HIS:CE1	2.56	0.40
1:A:267:THR:OG1	1:A:268:PRO:HA	2.21	0.40
1:B:247:GLU:CD	1:B:247:GLU:H	2.24	0.40
1:A:160:ILE:HD12	1:A:165:VAL:HG11	2.03	0.40
1:D:205:THR:O	1:D:205:THR:HG22	2.20	0.40
1:E:282:ARG:HG3	1:E:283:VAL:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:GLU:CG	1:E:151:ILE:HD11	2.25	0.40
1:C:196:SER:O	1:C:254:LYS:HE2	2.22	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	179/235 (76%)	167 (93%)	12 (7%)	0	100 100
1	B	183/235 (78%)	173 (94%)	8 (4%)	2 (1%)	14 20
1	C	172/235 (73%)	163 (95%)	8 (5%)	1 (1%)	25 36
1	D	182/235 (77%)	173 (95%)	5 (3%)	4 (2%)	6 7
1	E	173/235 (74%)	163 (94%)	7 (4%)	3 (2%)	9 11
All	All	889/1175 (76%)	839 (94%)	40 (4%)	10 (1%)	14 20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	124	SER
1	D	121	ASN
1	D	134	SER
1	D	137	PRO
1	E	123	GLU
1	E	133	GLU
1	B	124	SER
1	B	134	SER
1	D	256	PRO
1	E	284	PRO

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	161/208 (77%)	147 (91%)	14 (9%)	10 15
1	B	163/208 (78%)	143 (88%)	20 (12%)	4 6
1	C	156/208 (75%)	140 (90%)	16 (10%)	7 10
1	D	162/208 (78%)	147 (91%)	15 (9%)	9 13
1	E	157/208 (76%)	144 (92%)	13 (8%)	11 17
All	All	799/1040 (77%)	721 (90%)	78 (10%)	8 11

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	THR
1	A	108	ILE
1	A	123	GLU
1	A	127	ILE
1	A	128	LEU
1	A	141	GLN
1	A	146	LEU
1	A	176	ARG
1	A	220	LYS
1	A	224	VAL
1	A	230	LEU
1	A	249	THR
1	A	268	PRO
1	A	271	VAL
1	B	124	SER
1	B	127	ILE
1	B	134	SER
1	B	135	GLN
1	B	136	ARG
1	B	141	GLN
1	B	174	ASP
1	B	176	ARG
1	B	179	THR

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Mol	Chain	Res	Type
1	B	224	VAL
1	B	228	SER
1	B	230	LEU
1	B	244	VAL
1	B	249	THR
1	B	258	ARG
1	B	267	THR
1	B	282	ARG
1	B	283	VAL
1	B	285	MET
1	B	286	ASP
1	C	133	GLU
1	C	138	ASP
1	C	146	LEU
1	C	151	ILE
1	C	152	ASP
1	C	155	MET
1	C	176	ARG
1	C	179	THR
1	C	208	SER
1	C	224	VAL
1	C	230	LEU
1	C	245	LYS
1	C	247	GLU
1	C	253	ARG
1	C	258	ARG
1	C	271	VAL
1	D	106	GLU
1	D	116	GLU
1	D	133	GLU
1	D	135	GLN
1	D	136	ARG
1	D	141	GLN
1	D	146	LEU
1	D	155	MET
1	D	159	VAL
1	D	179	THR
1	D	230	LEU
1	D	244	VAL
1	D	249	THR
1	D	253	ARG
1	D	282	ARG

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Mol	Chain	Res	Type
1	E	107	THR
1	E	108	ILE
1	E	122	LEU
1	E	124	SER
1	E	197	THR
1	E	208	SER
1	E	209	THR
1	E	230	LEU
1	E	235	LYS
1	E	244	VAL
1	E	245	LYS
1	E	269	TYR
1	E	271	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	218	GLN
1	C	120	ASN
1	C	141	GLN
1	C	217	ASN
1	C	218	GLN
1	D	141	GLN
1	D	204	HIS
1	E	218	GLN

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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{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	181/235 (77%)	-0.32	1 (0%)	89	88	22, 39, 72, 99	0
1	B	185/235 (78%)	-0.48	1 (0%)	91	89	19, 32, 65, 106	0
1	C	176/235 (74%)	-0.21	0	100	100	25, 39, 73, 99	0
1	D	184/235 (78%)	-0.35	2 (1%)	80	79	23, 39, 70, 86	0
1	E	177/235 (75%)	-0.11	2 (1%)	80	79	32, 52, 86, 114	0
All	All	903/1175 (76%)	-0.30	6 (0%)	87	86	19, 40, 76, 114	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	GLN	3.5
1	D	134	SER	2.8
1	E	143	GLN	2.3
1	E	123	GLU	2.2
1	D	135	GLN	2.1
1	A	113	ALA	2.0

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

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	1287	1/1	0.85	0.21	72,72,72,72	0
2	CA	B	1288	1/1	0.88	0.09	71,71,71,71	0
2	CA	C	1286	1/1	0.92	0.07	66,66,66,66	0
2	CA	A	1286	1/1	0.99	0.05	44,44,44,44	0

6.5 Other polymers

There are no such residues in this entry.