



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:57 pm GMT

PDB ID : 3B8P
Title : Fragment of WzzB, Polysaccharide Co-polymerase from Salmonella Typhimurium
Authors : Tocilj, A.; Matte, A.; Cygler, M.
Deposited on : 2007-11-01
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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

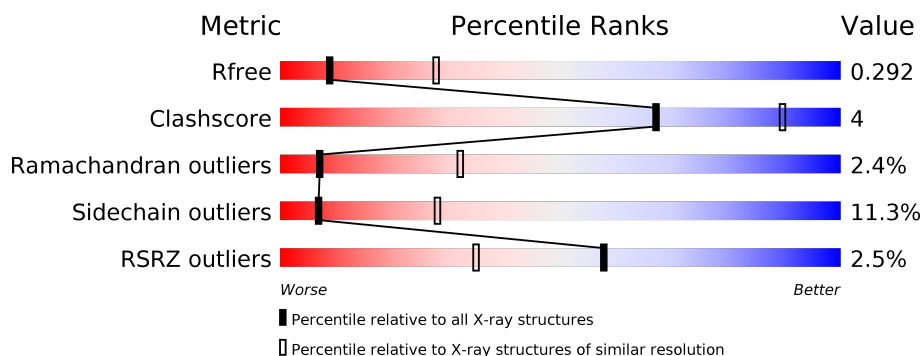
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 $\leq 5\%$. 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	243	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>••</div> <div>15%</div> </div> </div>
1	B	243	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>13%</div> <div>•</div> <div>28%</div> </div> </div>
1	C	243	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>12%</div> <div>•</div> <div>24%</div> </div> </div>
1	D	243	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>14%</div> <div>•</div> <div>24%</div> </div> </div>
1	E	243	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>12%</div> <div>•</div> <div>22%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6778 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 Chain length determinant protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	Se	0	0	0
			1482	924	251	306	1			
1	B	174	Total	C	N	O	Se	0	0	0
			1248	778	212	257	1			
1	C	185	Total	C	N	O	Se	0	0	0
			1393	878	230	284	1			
1	D	185	Total	C	N	O	Se	0	0	0
			1338	837	224	276	1			
1	E	189	Total	C	N	O	Se	0	0	0
			1317	825	214	277	1			

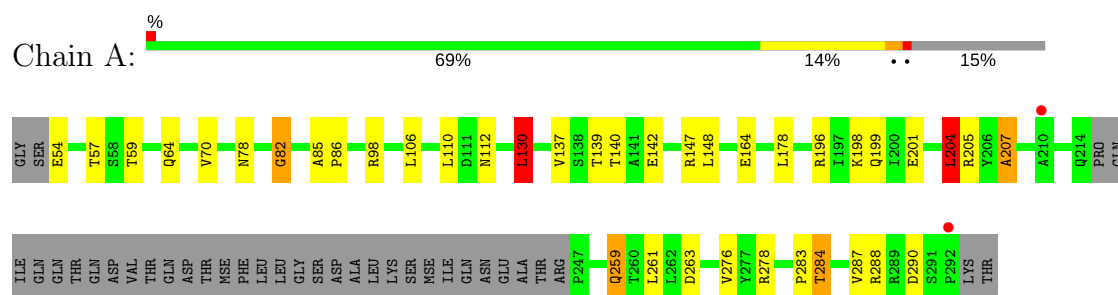
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLY	-	EXPRESSION TAG	UNP Q04866
A	53	SER	-	EXPRESSION TAG	UNP Q04866
B	52	GLY	-	EXPRESSION TAG	UNP Q04866
B	53	SER	-	EXPRESSION TAG	UNP Q04866
C	52	GLY	-	EXPRESSION TAG	UNP Q04866
C	53	SER	-	EXPRESSION TAG	UNP Q04866
D	52	GLY	-	EXPRESSION TAG	UNP Q04866
D	53	SER	-	EXPRESSION TAG	UNP Q04866
E	52	GLY	-	EXPRESSION TAG	UNP Q04866
E	53	SER	-	EXPRESSION TAG	UNP Q04866

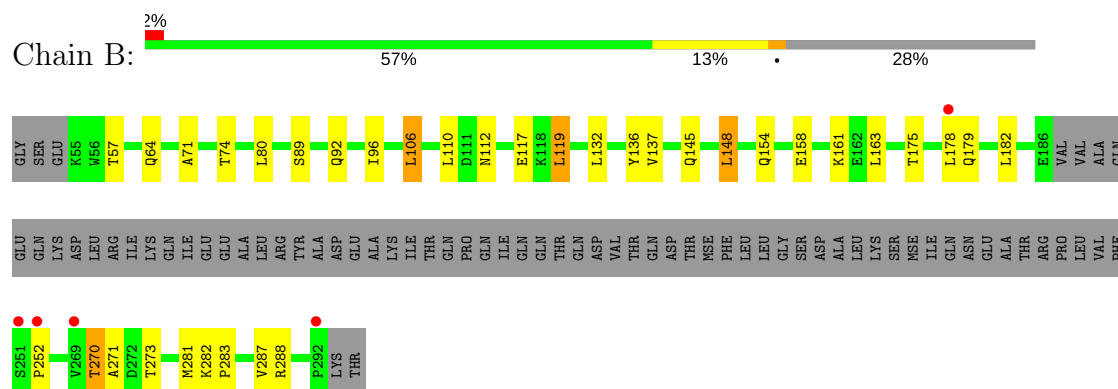
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

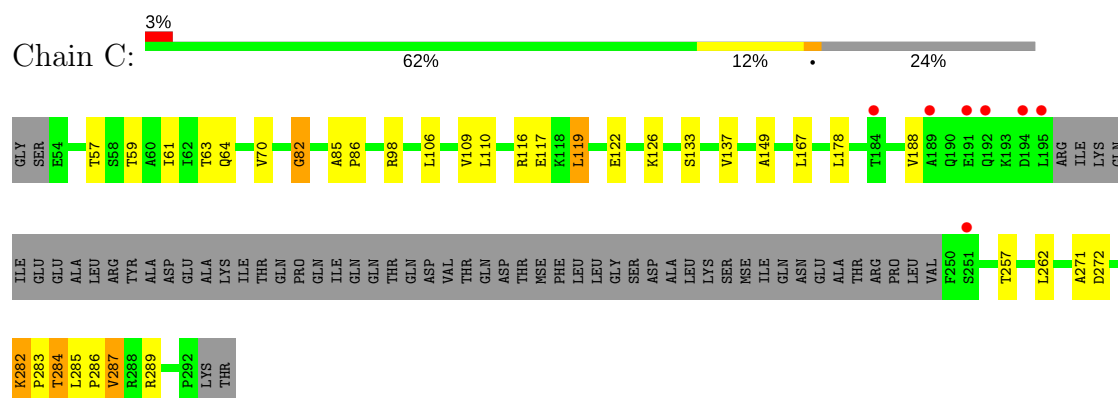
• Molecule 1: Chain length determinant protein



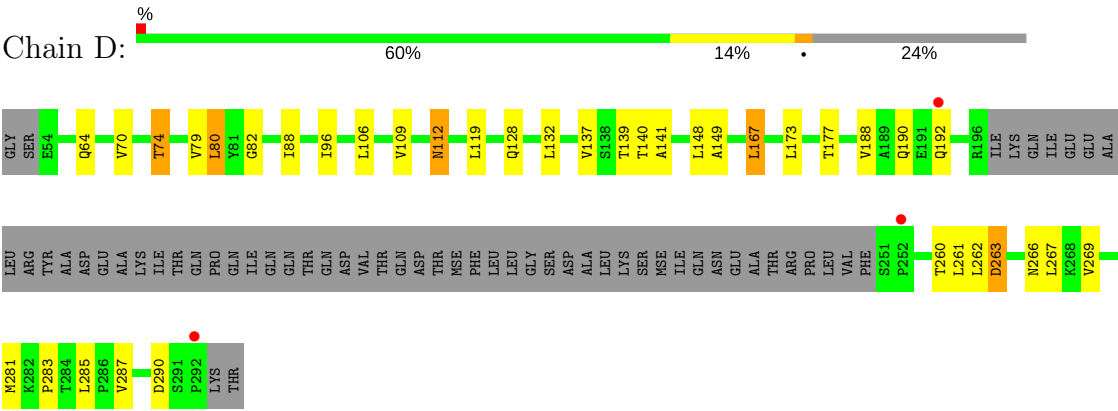
• Molecule 1: Chain length determinant protein



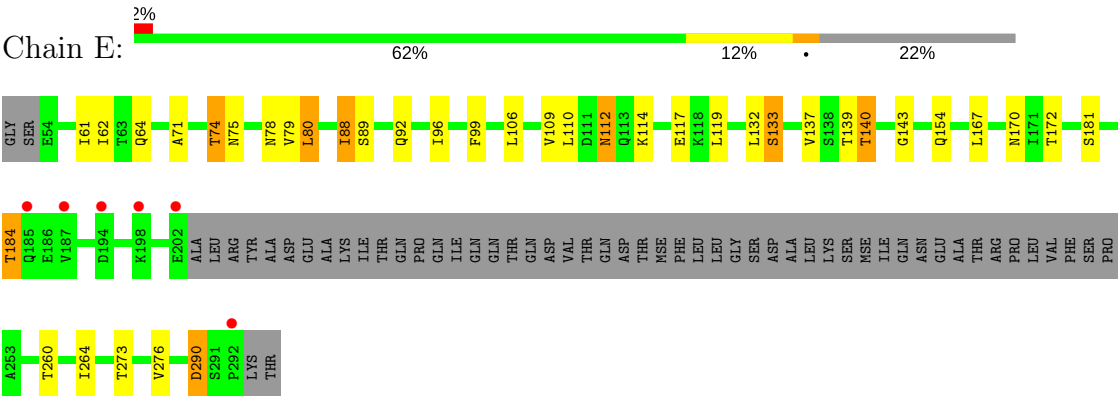
• Molecule 1: Chain length determinant protein



• Molecule 1: Chain length determinant protein



• Molecule 1: Chain length determinant protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.97Å 112.74Å 170.93Å 90.00° 97.34° 90.00°	Depositor
Resolution (Å)	29.24 – 3.10 29.28 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.24-3.10) 87.1 (29.28-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.255 , 0.301 0.245 , 0.292	Depositor DCC
R_{free} test set	1416 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6778	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.95	0/1500	1.12	5/2055 (0.2%)
1	B	0.95	0/1264	1.09	2/1736 (0.1%)
1	C	0.95	0/1412	1.12	4/1930 (0.2%)
1	D	0.95	0/1354	1.11	2/1856 (0.1%)
1	E	0.90	0/1333	1.12	3/1835 (0.2%)
All	All	0.94	0/6863	1.11	16/9412 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	290	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	204	LEU	CA-CB-CG	7.31	132.12	115.30
1	A	204	LEU	CB-CG-CD1	6.37	121.82	111.00
1	E	290	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	D	80	LEU	CA-CB-CG	5.87	128.80	115.30
1	C	82	GLY	N-CA-C	5.74	127.44	113.10
1	A	207	ALA	N-CA-C	5.68	126.33	111.00
1	A	130	LEU	CB-CG-CD1	5.42	120.22	111.00
1	B	163	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	B	80	LEU	CA-CB-CG	5.36	127.62	115.30
1	E	114	LYS	N-CA-C	-5.22	96.91	111.00
1	C	287	VAL	N-CA-C	-5.16	97.06	111.00
1	D	188	VAL	CB-CA-C	5.15	121.19	111.40
1	C	262	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	98	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	119	LEU	CA-CB-CG	5.04	126.90	115.30

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	1482	0	1334	14	0
1	B	1248	0	1134	14	0
1	C	1393	0	1328	11	0
1	D	1338	0	1244	12	0
1	E	1317	0	1155	14	0
All	All	6778	0	6195	58	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 4.

All (58) 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:89:SER:HA	1:E:92:GLN:HE21	1.51	0.74
1:A:59:THR:H	1:A:284:THR:HG22	1.55	0.70
1:E:61:ILE:HG12	1:E:133:SER:HB3	1.75	0.68
1:B:57:THR:HG22	1:B:137:VAL:HG22	1.78	0.63
1:D:64:GLN:HA	1:D:96:ILE:HB	1.82	0.60
1:B:281:MSE:HE1	1:D:109:VAL:HG23	1.83	0.59
1:B:287:VAL:H	1:D:112:ASN:HD21	1.50	0.58
1:B:89:SER:HA	1:B:92:GLN:HE21	1.69	0.57
1:E:181:SER:HA	1:E:184:THR:HG22	1.87	0.57
1:A:287:VAL:H	1:B:112:ASN:HD21	1.53	0.55
1:C:59:THR:H	1:C:284:THR:HG22	1.70	0.55
1:D:148:LEU:HD23	1:D:283:PRO:HB3	1.89	0.55
1:E:110:LEU:HB3	1:E:117:GLU:HB2	1.89	0.54
1:D:260:THR:C	1:D:262:LEU:H	2.11	0.53
1:E:99:PHE:HB2	1:E:276:VAL:HG12	1.91	0.52
1:C:110:LEU:HB3	1:C:117:GLU:HB2	1.91	0.52
1:D:74:THR:HG21	1:D:88:ILE:HG22	1.91	0.51
1:A:112:ASN:HD21	1:C:287:VAL:H	1.58	0.51
1:B:110:LEU:HD12	1:B:119:LEU:HB2	1.93	0.51
1:D:281:MSE:SE	1:E:109:VAL:HG23	2.61	0.51
1:D:260:THR:O	1:D:262:LEU:N	2.43	0.51
1:A:148:LEU:HD23	1:A:283:PRO:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:HG22	1:A:140:THR:HG23	1.94	0.50
1:C:149:ALA:HB2	1:C:283:PRO:HG2	1.94	0.49
1:A:196:ARG:HA	1:A:199:GLN:HG2	1.93	0.49
1:E:140:THR:HG23	1:E:143:GLY:HA3	1.94	0.49
1:A:78:ASN:O	1:A:82:GLY:N	2.39	0.48
1:C:61:ILE:HG12	1:C:133:SER:HB3	1.93	0.48
1:D:287:VAL:H	1:E:112:ASN:HD21	1.61	0.48
1:B:270:THR:HG23	1:B:273:THR:HG23	1.96	0.48
1:E:64:GLN:HA	1:E:96:ILE:HB	1.96	0.48
1:A:57:THR:HG22	1:A:137:VAL:HG22	1.95	0.47
1:E:79:VAL:HG12	1:E:80:LEU:HD23	1.96	0.46
1:B:117:GLU:OE1	1:B:136:TYR:OH	2.25	0.46
1:B:106:LEU:HD22	1:B:110:LEU:HG	1.97	0.46
1:A:198:LYS:HA	1:A:201:GLU:HB3	1.99	0.45
1:C:178:LEU:HD22	1:C:257:THR:HG23	1.97	0.45
1:A:112:ASN:HD21	1:C:286:PRO:HA	1.81	0.44
1:A:64:GLN:HB3	1:A:130:LEU:HD21	2.00	0.44
1:B:179:GLN:HA	1:B:182:LEU:HD12	2.00	0.43
1:E:74:THR:HG21	1:E:88:ILE:HG23	1.99	0.43
1:A:259:GLN:HB3	1:A:259:GLN:HE21	1.64	0.43
1:B:64:GLN:HA	1:B:96:ILE:HB	2.00	0.43
1:D:263:ASP:N	1:D:263:ASP:OD1	2.52	0.43
1:E:260:THR:O	1:E:264:ILE:HG13	2.19	0.43
1:A:178:LEU:HB3	1:A:261:LEU:HD22	2.00	0.42
1:C:63:THR:OG1	1:C:64:GLN:N	2.51	0.42
1:A:85:ALA:HA	1:A:86:PRO:HD2	1.80	0.42
1:E:112:ASN:HD22	1:E:112:ASN:HA	1.56	0.41
1:E:75:ASN:HA	1:E:78:ASN:HD22	1.85	0.41
1:B:148:LEU:HD13	1:B:283:PRO:HB3	2.03	0.41
1:D:167:LEU:HD13	1:D:269:VAL:HG11	2.03	0.41
1:B:175:THR:HA	1:B:178:LEU:HD12	2.03	0.41
1:C:282:LYS:H	1:C:282:LYS:HD2	1.86	0.41
1:C:122:GLU:OE1	1:C:126:LYS:NZ	2.41	0.41
1:B:281:MSE:HE3	1:B:281:MSE:HB2	1.98	0.40
1:D:149:ALA:HB2	1:D:283:PRO:HG2	2.03	0.40
1:C:85:ALA:HA	1:C:86:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

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	203/243 (84%)	179 (88%)	19 (9%)	5 (2%)	6	31
1	B	170/243 (70%)	153 (90%)	13 (8%)	4 (2%)	7	32
1	C	181/243 (74%)	161 (89%)	17 (9%)	3 (2%)	11	42
1	D	181/243 (74%)	154 (85%)	18 (10%)	9 (5%)	2	16
1	E	185/243 (76%)	171 (92%)	13 (7%)	1 (0%)	32	71
All	All	920/1215 (76%)	818 (89%)	80 (9%)	22 (2%)	7	32

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	B	71	ALA
1	C	82	GLY
1	D	261	LEU
1	A	82	GLY
1	A	205	ARG
1	A	207	ALA
1	C	116	ARG
1	D	266	ASN
1	D	267	LEU
1	D	290	ASP
1	B	145	GLN
1	B	252	PRO
1	C	271	ALA
1	D	139	THR
1	A	288	ARG
1	D	79	VAL
1	D	80	LEU
1	D	141	ALA
1	B	271	ALA
1	E	71	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	82	GLY

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	140/212 (66%)	125 (89%)	15 (11%)	8	30
1	B	121/212 (57%)	110 (91%)	11 (9%)	11	39
1	C	145/212 (68%)	131 (90%)	14 (10%)	9	35
1	D	134/212 (63%)	118 (88%)	16 (12%)	6	25
1	E	123/212 (58%)	104 (85%)	19 (15%)	3	14
All	All	663/1060 (62%)	588 (89%)	75 (11%)	7	28

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	70	VAL
1	A	106	LEU
1	A	110	LEU
1	A	130	LEU
1	A	142	GLU
1	A	147	ARG
1	A	164	GLU
1	A	204	LEU
1	A	259	GLN
1	A	263	ASP
1	A	276	VAL
1	A	278	ARG
1	A	284	THR
1	A	290	ASP
1	B	74	THR
1	B	106	LEU
1	B	119	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	132	LEU
1	B	148	LEU
1	B	154	GLN
1	B	158	GLU
1	B	161	LYS
1	B	270	THR
1	B	282	LYS
1	B	288	ARG
1	C	57	THR
1	C	70	VAL
1	C	98	ARG
1	C	106	LEU
1	C	109	VAL
1	C	119	LEU
1	C	137	VAL
1	C	167	LEU
1	C	188	VAL
1	C	272	ASP
1	C	282	LYS
1	C	284	THR
1	C	285	LEU
1	C	289	ARG
1	D	70	VAL
1	D	74	THR
1	D	106	LEU
1	D	112	ASN
1	D	119	LEU
1	D	128	GLN
1	D	132	LEU
1	D	137	VAL
1	D	140	THR
1	D	167	LEU
1	D	173	LEU
1	D	177	THR
1	D	190	GLN
1	D	192	GLN
1	D	263	ASP
1	D	285	LEU
1	E	62	ILE
1	E	74	THR
1	E	80	LEU
1	E	88	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	106	LEU
1	E	112	ASN
1	E	119	LEU
1	E	132	LEU
1	E	133	SER
1	E	137	VAL
1	E	139	THR
1	E	140	THR
1	E	154	GLN
1	E	167	LEU
1	E	170	ASN
1	E	172	THR
1	E	184	THR
1	E	273	THR
1	E	290	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	128	GLN
1	A	259	GLN
1	B	69	GLN
1	B	92	GLN
1	B	112	ASN
1	B	113	GLN
1	C	78	ASN
1	C	112	ASN
1	C	123	GLN
1	D	69	GLN
1	D	112	ASN
1	D	123	GLN
1	D	128	GLN
1	D	190	GLN
1	E	78	ASN
1	E	92	GLN
1	E	94	ASN
1	E	112	ASN
1	E	145	GLN
1	E	174	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 carbohydrates 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

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, 95th 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	206/243 (84%)	-0.39	2 (0%) 82 67	13, 62, 109, 117	0
1	B	173/243 (71%)	-0.23	5 (2%) 52 28	16, 59, 119, 120	0
1	C	184/243 (75%)	-0.26	7 (3%) 41 20	16, 57, 118, 120	0
1	D	184/243 (75%)	-0.36	3 (1%) 72 51	15, 55, 120, 120	0
1	E	188/243 (77%)	-0.24	6 (3%) 48 25	20, 60, 120, 120	0
All	All	935/1215 (76%)	-0.30	23 (2%) 58 35	13, 58, 119, 120	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	PRO	4.0
1	C	195	LEU	3.8
1	B	269	VAL	3.6
1	D	292	PRO	3.6
1	E	194	ASP	3.4
1	C	194	ASP	3.1
1	E	202	GLU	3.0
1	C	251	SER	3.0
1	E	292	PRO	3.0
1	C	189	ALA	2.9
1	D	192	GLN	2.9
1	A	210	ALA	2.7
1	B	252	PRO	2.7
1	B	292	PRO	2.7
1	E	198	LYS	2.6
1	B	178	LEU	2.4
1	E	185	GLN	2.3
1	C	184	THR	2.2
1	C	192	GLN	2.2
1	B	251	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	252	PRO	2.1
1	C	191	GLU	2.1
1	E	187	VAL	2.1

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 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.