



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:32 PM UTC

PDB ID : 6PL5 / pdb_00006pl5
Title : Structural coordination of polymerization and crosslinking by a peptidoglycan synthase complex
Authors : Sjodt, M.; Rohs, P.D.A.; Erlandson, S.C.; Zheng, S.; Rudner, D.Z.; Bernhardt, T.G.; Kruse, A.C.
Deposited on : 2019-06-30
Resolution : 3.50 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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

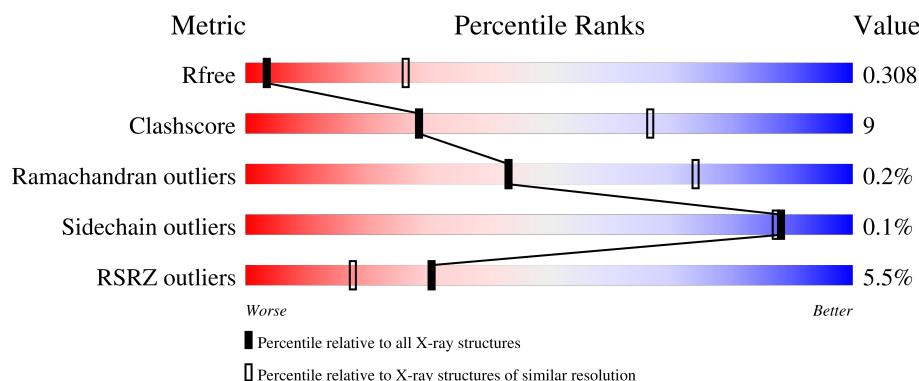
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 $\leq 5\%$. 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	377	5% 77% 12% 11%
2	B	598	5% 72% 24%
3	D	11	100%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6843 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 Peptidoglycan glycosyltransferase RodA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2513	1692	411	407	3			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	ASP	-	expression tag	UNP Q5SIX3
A	-16	TYR	-	expression tag	UNP Q5SIX3
A	-15	LYS	-	expression tag	UNP Q5SIX3
A	-14	ASP	-	expression tag	UNP Q5SIX3
A	-13	ASP	-	expression tag	UNP Q5SIX3
A	-12	ASP	-	expression tag	UNP Q5SIX3
A	-11	ASP	-	expression tag	UNP Q5SIX3
A	-10	LEU	-	expression tag	UNP Q5SIX3
A	-9	GLU	-	expression tag	UNP Q5SIX3
A	-8	VAL	-	expression tag	UNP Q5SIX3
A	-7	LEU	-	expression tag	UNP Q5SIX3
A	-6	PHE	-	expression tag	UNP Q5SIX3
A	-5	GLN	-	expression tag	UNP Q5SIX3
A	-4	GLY	-	expression tag	UNP Q5SIX3
A	-3	PRO	-	expression tag	UNP Q5SIX3
A	-2	GLY	-	expression tag	UNP Q5SIX3
A	-1	GLY	-	expression tag	UNP Q5SIX3
A	0	SER	-	expression tag	UNP Q5SIX3
A	1	SER	-	expression tag	UNP Q5SIX3

- Molecule 2 is a protein called Penicillin-binding protein 2/cell division protein FtsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	577	Total	C	N	O	S	0	0	0
			4275	2737	742	787	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP Q5SJ23
B	1	GLY	-	expression tag	UNP Q5SJ23
B	576	GLY	-	expression tag	UNP Q5SJ23
B	577	SER	-	expression tag	UNP Q5SJ23
B	578	LEU	-	expression tag	UNP Q5SJ23
B	579	GLU	-	expression tag	UNP Q5SJ23
B	580	VAL	-	expression tag	UNP Q5SJ23
B	581	LEU	-	expression tag	UNP Q5SJ23
B	582	PHE	-	expression tag	UNP Q5SJ23
B	583	GLN	-	expression tag	UNP Q5SJ23
B	584	GLY	-	expression tag	UNP Q5SJ23
B	585	PRO	-	expression tag	UNP Q5SJ23
B	586	GLU	-	expression tag	UNP Q5SJ23
B	587	ASP	-	expression tag	UNP Q5SJ23
B	588	GLN	-	expression tag	UNP Q5SJ23
B	589	VAL	-	expression tag	UNP Q5SJ23
B	590	ASP	-	expression tag	UNP Q5SJ23
B	591	PRO	-	expression tag	UNP Q5SJ23
B	592	ARG	-	expression tag	UNP Q5SJ23
B	593	LEU	-	expression tag	UNP Q5SJ23
B	594	ILE	-	expression tag	UNP Q5SJ23
B	595	ASP	-	expression tag	UNP Q5SJ23
B	596	GLY	-	expression tag	UNP Q5SJ23
B	597	LYS	-	expression tag	UNP Q5SJ23

- Molecule 3 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	0	0	0
			55	33	11	11			

- Molecule 3: Unknown peptide

Chain D:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.57Å 119.57Å 267.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.77 – 3.50 44.77 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.2 (44.77-3.50) 79.1 (44.77-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.40 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.285 , 0.305 0.289 , 0.308	Depositor DCC
R_{free} test set	1870 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å ²)	127.2	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 124.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6843	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.10	0/2576	0.31	2/3529 (0.1%)
2	B	0.10	0/4372	0.29	0/5980
All	All	0.10	0/6948	0.30	2/9509 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	PRO	CB-CA-C	6.62	122.48	111.56
1	A	332	PHE	N-CA-C	-5.34	108.54	114.62

There are no chirality outliers.

There are no planarity outliers.

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	2513	0	2628	33	0
2	B	4275	0	4218	91	0
3	D	55	0	13	0	0
All	All	6843	0	6859	121	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 9.

All (121) 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)
2:B:168:ALA:HB3	2:B:171:GLU:HB2	1.67	0.75
2:B:230:LEU:HD11	2:B:246:LYS:HA	1.69	0.74
2:B:332:CYS:HB3	2:B:351:MET:HB2	1.71	0.73
1:A:173:PRO:HG2	1:A:177:LEU:HB2	1.72	0.71
1:A:229:GLY:O	2:B:27:GLN:NE2	2.25	0.69
1:A:257:VAL:HG21	1:A:333:SER:HA	1.75	0.69
2:B:48:ILE:HG12	2:B:185:ARG:HH21	1.59	0.68
2:B:218:LEU:HB3	2:B:264:ALA:HB2	1.74	0.68
1:A:33:ALA:HB2	1:A:260:VAL:HG11	1.75	0.67
2:B:75:THR:O	2:B:124:ASN:ND2	2.29	0.66
2:B:516:ALA:HB3	2:B:527:HIS:HB2	1.79	0.64
2:B:135:TYR:H	2:B:274:ASN:HD21	1.46	0.63
1:A:227:ALA:HB2	2:B:26:LEU:HB3	1.81	0.61
2:B:399:GLU:N	2:B:399:GLU:OE1	2.33	0.61
1:A:62:ARG:NH2	1:A:295:SER:OG	2.34	0.60
2:B:133:ARG:HD3	2:B:147:VAL:HG21	1.83	0.60
2:B:262:VAL:HG21	2:B:461:LEU:HD23	1.83	0.59
2:B:299:ARG:NH1	2:B:551:GLU:OE2	2.35	0.59
2:B:308:SER:HB2	2:B:514:GLY:HA2	1.84	0.59
1:A:26:GLY:HA2	1:A:332:PHE:CD1	2.38	0.58
1:A:330:PRO:O	1:A:332:PHE:N	2.36	0.58
2:B:447:LEU:HD23	2:B:545:VAL:HG13	1.87	0.56
2:B:190:ASN:OD1	2:B:191:VAL:N	2.37	0.56
2:B:254:ALA:HB3	2:B:264:ALA:HB3	1.88	0.55
2:B:379:PHE:O	2:B:383:LEU:N	2.39	0.54
2:B:294:LEU:HD13	2:B:297:LEU:HD12	1.89	0.54
2:B:449:THR:HG22	2:B:456:LYS:HA	1.89	0.53
2:B:133:ARG:NE	2:B:171:GLU:OE2	2.39	0.53
2:B:337:VAL:HG22	2:B:342:VAL:HG22	1.89	0.53
2:B:501:VAL:HG13	2:B:565:ARG:HD2	1.90	0.53
1:A:273:LEU:HD11	1:A:277:TYR:HE1	1.74	0.52
2:B:141:GLY:O	2:B:145:GLY:N	2.42	0.52
2:B:151:ASN:OD1	2:B:152:ALA:N	2.42	0.52
1:A:329:LEU:HD12	1:A:330:PRO:HD2	1.92	0.52
2:B:229:ALA:O	2:B:233:ILE:N	2.36	0.52
2:B:74:TYR:HE1	2:B:77:GLY:HA2	1.75	0.51
2:B:389:LEU:HD21	2:B:478:PRO:HD2	1.92	0.51
2:B:145:GLY:HA3	2:B:168:ALA:HB1	1.91	0.51
2:B:564:VAL:HG12	2:B:568:MET:HE2	1.93	0.51
1:A:65:LEU:HD22	1:A:351:LEU:HD23	1.93	0.50
2:B:318:LEU:HD21	2:B:371:ALA:HB1	1.92	0.50
2:B:369:TYR:HA	2:B:427:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:THR:HB	2:B:261:GLU:HB3	1.92	0.50
1:A:105:GLN:HG2	1:A:107:LEU:H	1.76	0.49
2:B:414:ARG:HA	2:B:420:PRO:HD2	1.93	0.49
2:B:493:VAL:HA	2:B:498:ALA:HB3	1.94	0.49
1:A:218:GLY:O	1:A:222:ILE:HG12	2.13	0.49
2:B:54:LYS:HG2	2:B:65:GLN:HG3	1.94	0.49
2:B:462:VAL:HG11	2:B:465:ILE:HG13	1.95	0.48
2:B:537:ASP:OD1	2:B:538:GLY:N	2.46	0.48
2:B:116:GLU:O	2:B:119:THR:OG1	2.31	0.48
2:B:312:LEU:HD21	2:B:489:LEU:HD11	1.95	0.47
2:B:146:TYR:HB2	2:B:276:PHE:HB2	1.96	0.47
2:B:502:LEU:HA	2:B:505:PHE:HB2	1.96	0.47
1:A:173:PRO:O	1:A:177:LEU:N	2.42	0.47
2:B:377:LEU:HD21	2:B:423:PRO:HB3	1.96	0.47
2:B:336:ILE:HD13	2:B:370:GLN:HG3	1.97	0.47
2:B:500:PHE:CD2	2:B:501:VAL:HG23	2.50	0.47
2:B:184:VAL:H	2:B:202:GLU:HB3	1.79	0.46
2:B:303:PRO:HB2	2:B:437:LEU:HB3	1.97	0.46
2:B:428:SER:HB3	2:B:433:GLN:HB3	1.97	0.46
2:B:72:LEU:HB2	2:B:103:LEU:O	2.14	0.46
2:B:68:LEU:HD22	2:B:129:GLU:HB3	1.97	0.46
1:A:42:ARG:HB2	1:A:334:TYR:OH	2.14	0.46
1:A:232:GLY:H	1:A:266:GLY:HA3	1.80	0.46
2:B:170:LEU:HD21	2:B:212:LEU:HD11	1.98	0.46
2:B:316:TYR:CE2	2:B:386:ARG:HB3	2.51	0.46
2:B:479:GLY:HA3	2:B:482:TRP:CE2	2.51	0.46
2:B:22:ARG:NH2	2:B:25:GLN:OE1	2.49	0.46
2:B:73:VAL:HG22	2:B:102:VAL:HG22	1.97	0.46
2:B:361:ALA:HA	2:B:492:THR:OG1	2.15	0.46
2:B:330:TYR:HB2	2:B:367:TRP:CE3	2.51	0.45
2:B:332:CYS:SG	2:B:366:THR:OG1	2.74	0.45
1:A:43:GLN:HB2	1:A:334:TYR:CE1	2.52	0.45
2:B:400:VAL:HG23	2:B:461:LEU:HD11	1.98	0.45
1:A:253:HIS:O	1:A:257:VAL:HG22	2.17	0.45
2:B:48:ILE:HD11	2:B:185:ARG:HB3	1.98	0.44
2:B:380:VAL:HG21	2:B:421:TRP:CH2	2.51	0.44
2:B:55:ILE:HD12	2:B:144:MET:HE1	1.99	0.44
1:A:121:ALA:HB1	1:A:135:LEU:HD21	1.99	0.44
2:B:145:GLY:HA3	2:B:168:ALA:CB	2.47	0.44
2:B:534:GLY:N	2:B:544:LEU:O	2.51	0.44
2:B:364:CYS:SG	2:B:366:THR:OG1	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:LEU:HD22	2:B:459:LEU:HD22	2.00	0.43
2:B:261:GLU:OE2	2:B:463:LYS:NZ	2.51	0.43
2:B:544:LEU:HD22	2:B:571:TYR:CG	2.53	0.43
1:A:128:ALA:HA	1:A:132:ASP:HB2	2.00	0.43
2:B:218:LEU:HD11	2:B:571:TYR:CD1	2.54	0.43
1:A:315:LEU:HB2	2:B:19:LEU:HD13	2.01	0.43
1:A:330:PRO:C	1:A:332:PHE:H	2.26	0.43
2:B:47:ASP:HA	2:B:184:VAL:HA	1.99	0.43
2:B:361:ALA:HB2	2:B:491:LYS:HB3	2.00	0.43
2:B:392:LEU:HD12	2:B:392:LEU:HA	1.90	0.43
2:B:550:PHE:HE2	2:B:560:ALA:HA	1.83	0.43
1:A:18:LEU:O	1:A:22:ILE:HG13	2.19	0.42
1:A:26:GLY:HA2	1:A:332:PHE:HD1	1.79	0.42
1:A:203:ARG:O	1:A:207:VAL:HG23	2.19	0.42
2:B:86:LEU:HB2	2:B:87:PRO:HD3	2.00	0.42
2:B:505:PHE:CZ	2:B:574:ILE:HG13	2.55	0.42
1:A:273:LEU:HD11	1:A:277:TYR:CE1	2.54	0.42
1:A:42:ARG:HA	1:A:45:VAL:HG22	2.02	0.42
2:B:403:LYS:HD2	2:B:403:LYS:HA	1.91	0.42
2:B:135:TYR:H	2:B:274:ASN:ND2	2.14	0.42
2:B:119:THR:HA	2:B:125:LEU:HD23	2.00	0.41
2:B:63:LEU:HD13	2:B:139:ILE:HD12	2.01	0.41
2:B:431:ILE:HD11	2:B:433:GLN:HB2	2.02	0.41
2:B:326:PRO:HB3	2:B:484:VAL:HG21	2.02	0.41
2:B:203:GLU:OE1	2:B:203:GLU:N	2.45	0.41
1:A:123:GLU:HA	1:A:294:LEU:HD23	2.02	0.41
1:A:166:VAL:HG13	1:A:298:LEU:HD22	2.02	0.41
1:A:188:VAL:HB	1:A:189:PRO:HD3	2.02	0.41
1:A:315:LEU:HD21	1:A:329:LEU:HD22	2.03	0.41
2:B:55:ILE:HB	2:B:64:ALA:HB3	2.03	0.40
1:A:266:GLY:O	1:A:270:VAL:HG23	2.21	0.40
2:B:336:ILE:O	2:B:343:ARG:N	2.41	0.40
1:A:170:ARG:HD3	1:A:294:LEU:HD21	2.03	0.40
2:B:67:ARG:HG2	2:B:68:LEU:H	1.86	0.40
2:B:139:ILE:HD13	2:B:219:GLN:HG2	2.03	0.40
2:B:268:ALA:HA	2:B:270:SER:N	2.37	0.40
2:B:330:TYR:HB2	2:B:367:TRP:CZ3	2.56	0.40
2:B:514:GLY:HA3	2:B:529:TRP:HB2	2.04	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	332/377 (88%)	313 (94%)	17 (5%)	2 (1%)	21	54
2	B	573/598 (96%)	535 (93%)	38 (7%)	0	100	100
All	All	905/975 (93%)	848 (94%)	55 (6%)	2 (0%)	43	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	LEU
1	A	330	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	252/294 (86%)	251 (100%)	1 (0%)	84	81
2	B	416/471 (88%)	416 (100%)	0	100	100
All	All	668/765 (87%)	667 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	124	ASN
2	B	274	ASN
2	B	302	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 oligosaccharides 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	336/377 (89%)	0.54	19 (5%)	29 17	109, 169, 265, 400	0
2	B	577/598 (96%)	0.52	31 (5%)	31 18	116, 167, 242, 352	0
3	D	0/11	-	-	-	-	-
All	All	913/986 (92%)	0.53	50 (5%)	30 18	109, 167, 252, 400	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	373	ALA	4.6
1	A	225	THR	4.4
2	B	241	GLY	4.3
2	B	1	GLY	4.3
1	A	253	HIS	4.3
1	A	250	PRO	4.1
2	B	425	GLU	4.0
1	A	251	PHE	3.5
2	B	169	GLY	3.4
2	B	434	GLY	3.4
1	A	127	ILE	3.4
2	B	79	VAL	3.2
1	A	359	ASP	3.1
1	A	112	LEU	3.1
1	A	218	GLY	3.0
2	B	513	THR	2.8
2	B	357	ARG	2.7
2	B	43	LEU	2.7
2	B	431	ILE	2.5
1	A	153	LEU	2.5
1	A	228	ILE	2.5
2	B	447	LEU	2.5
1	A	21	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	374	GLN	2.4
2	B	159	TYR	2.4
2	B	90	GLY	2.4
1	A	164	PHE	2.3
2	B	148	LEU	2.3
1	A	86	VAL	2.3
1	A	215	LEU	2.3
2	B	215	ASP	2.3
2	B	376	PRO	2.3
2	B	329	THR	2.3
2	B	379	PHE	2.3
2	B	66	ASP	2.3
1	A	334	TYR	2.2
2	B	31	TYR	2.2
1	A	284	LEU	2.2
2	B	406	LEU	2.2
2	B	194	GLU	2.1
1	A	41	TYR	2.1
2	B	243	PRO	2.1
1	A	167	VAL	2.1
2	B	87	PRO	2.1
2	B	435	ALA	2.1
2	B	443	ILE	2.1
2	B	257	PRO	2.1
2	B	45	THR	2.0
1	A	124	GLY	2.0
2	B	308	SER	2.0

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 oligosaccharides 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.