



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:05 AM UTC

PDB ID : 3WDO / pdb_00003wdo
Title : Structure of E. coli YajR transporter
Authors : Jiang, D.
Deposited on : 2013-06-19
Resolution : 3.15 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

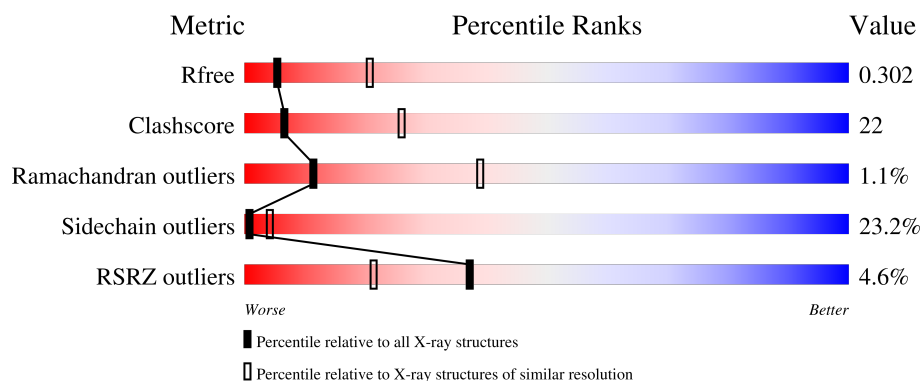
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	453	5% 50% 36% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3419 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 MFS Transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	453	3419	2243	560	594	22	0	0	0

3 Residue-property plots

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: MFS Transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.72Å 128.72Å 165.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.17 – 3.15 39.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.17-3.15) 99.3 (39.17-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.271 , 0.290 0.275 , 0.302	Depositor DCC
R_{free} test set	708 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3419	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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	0.75	1/3491 (0.0%)	1.30	24/4737 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ASP	CA-C	-5.37	1.48	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	THR	CA-C-N	-10.74	106.42	119.84
1	A	7	THR	C-N-CA	-10.74	106.42	119.84
1	A	78	LYS	CA-C-N	-8.54	111.02	119.64
1	A	78	LYS	C-N-CA	-8.54	111.02	119.64
1	A	77	ARG	N-CA-C	-8.46	101.89	112.72
1	A	41	ALA	N-CA-C	-7.65	97.51	108.07
1	A	73	ASP	N-CA-C	-7.60	101.71	112.13
1	A	264	VAL	CA-C-N	-7.16	115.73	120.24
1	A	264	VAL	C-N-CA	-7.16	115.73	120.24
1	A	39	GLY	N-CA-C	-7.12	103.74	111.93
1	A	265	VAL	CB-CA-C	-7.08	106.84	114.35
1	A	29	PHE	N-CA-C	6.97	118.53	111.07
1	A	390	GLU	CA-C-N	6.81	127.39	120.38
1	A	390	GLU	C-N-CA	6.81	127.39	120.38
1	A	211	GLU	CA-C-N	6.74	126.53	119.05
1	A	211	GLU	C-N-CA	6.74	126.53	119.05
1	A	202	LYS	N-CA-C	-6.59	104.83	114.39
1	A	213	ARG	CB-CG-CD	-5.72	98.15	111.30
1	A	208	VAL	N-CA-C	5.59	116.36	110.72
1	A	188	ASN	N-CA-C	5.45	118.22	107.98
1	A	424	VAL	N-CA-C	5.24	115.81	108.17
1	A	98	SER	N-CA-C	5.14	117.88	110.28
1	A	273	VAL	N-CA-C	5.12	115.78	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	MET	N-CA-C	-5.04	105.68	111.07

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	3419	0	3557	151	0
All	All	3419	0	3557	151	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 22.

All (151) 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:A:276:LYS:HB3	1:A:279:GLN:HG3	1.58	0.84
1:A:46:SER:HB3	1:A:49:LEU:HB2	1.60	0.81
1:A:66:ILE:HD13	1:A:66:ILE:H	1.46	0.79
1:A:7:THR:HG22	1:A:8:PRO:HD2	1.68	0.73
1:A:331:SER:HB2	1:A:336:LYS:HE2	1.70	0.71
1:A:52:ILE:HG22	1:A:105:ILE:HD11	1.74	0.70
1:A:245:PRO:HD2	1:A:248:GLU:HB2	1.76	0.68
1:A:102:TRP:HA	1:A:105:ILE:HG22	1.76	0.68
1:A:20:VAL:HG12	1:A:181:LEU:HD23	1.77	0.67
1:A:30:MET:HE2	1:A:155:GLY:HA2	1.76	0.67
1:A:26:LEU:O	1:A:30:MET:HG3	1.95	0.67
1:A:98:SER:OG	1:A:103:GLY:HA3	1.94	0.67
1:A:56:ILE:HD13	1:A:109:ALA:HB2	1.77	0.67
1:A:302:PHE:HE1	1:A:303:TRP:CE2	2.15	0.65
1:A:394:VAL:HA	1:A:437:ILE:O	1.97	0.64
1:A:10:GLU:OE1	1:A:132:ASN:ND2	2.31	0.63
1:A:66:ILE:HG12	1:A:67:PRO:HD3	1.80	0.62
1:A:27:GLY:O	1:A:31:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:NH1	1:A:440:LYS:HA	2.15	0.60
1:A:155:GLY:O	1:A:159:THR:HG22	2.01	0.59
1:A:234:ALA:HB2	1:A:370:VAL:CG2	2.33	0.59
1:A:255:ALA:O	1:A:259:ILE:HG12	2.02	0.58
1:A:54:ILE:HA	1:A:108:ARG:HE	1.68	0.58
1:A:34:VAL:HG22	1:A:159:THR:HG21	1.85	0.58
1:A:205:PHE:O	1:A:208:VAL:HG12	2.04	0.57
1:A:30:MET:CE	1:A:154:LEU:HG	2.34	0.56
1:A:53:ALA:O	1:A:56:ILE:HG22	2.05	0.56
1:A:234:ALA:HB2	1:A:370:VAL:HG21	1.86	0.56
1:A:91:GLY:HA3	1:A:110:LEU:HB2	1.88	0.56
1:A:373:ALA:HA	1:A:376:MET:HE2	1.88	0.56
1:A:423:GLU:HB3	1:A:436:LYS:HB2	1.88	0.56
1:A:10:GLU:OE2	1:A:129:ARG:N	2.33	0.55
1:A:7:THR:CB	1:A:10:GLU:HG3	2.37	0.55
1:A:121:MET:HE3	1:A:140:ILE:HD12	1.89	0.55
1:A:438:ASP:OD1	1:A:440:LYS:HB2	2.07	0.54
1:A:40:MET:HG2	1:A:45:ALA:HB1	1.90	0.54
1:A:7:THR:HB	1:A:10:GLU:HG3	1.89	0.54
1:A:40:MET:HA	1:A:45:ALA:HB1	1.91	0.53
1:A:82:VAL:HG13	1:A:179:ILE:HG23	1.90	0.53
1:A:326:LEU:HD22	1:A:391:PRO:HG3	1.91	0.53
1:A:303:TRP:O	1:A:307:VAL:HG12	2.07	0.53
1:A:242:ALA:HB2	1:A:300:THR:HA	1.90	0.53
1:A:226:MET:HA	1:A:354:GLY:HA3	1.89	0.53
1:A:40:MET:HG2	1:A:45:ALA:O	2.09	0.53
1:A:213:ARG:HD3	1:A:330:GLU:OE1	2.09	0.53
1:A:387:THR:O	1:A:387:THR:OG1	2.27	0.52
1:A:154:LEU:O	1:A:158:ILE:HG22	2.10	0.52
1:A:197:GLU:OE1	1:A:201:VAL:HA	2.09	0.52
1:A:271:ALA:HB2	1:A:280:VAL:HG21	1.91	0.52
1:A:150:ILE:HG22	1:A:154:LEU:HD23	1.91	0.51
1:A:390:GLU:HG3	1:A:391:PRO:HD2	1.91	0.51
1:A:124:LEU:HD11	1:A:136:ALA:HB1	1.92	0.51
1:A:247:ALA:O	1:A:250:TRP:CD1	2.64	0.51
1:A:30:MET:HE2	1:A:155:GLY:CA	2.41	0.51
1:A:385:ALA:O	1:A:388:MET:HG3	2.11	0.51
1:A:380:VAL:O	1:A:384:VAL:HG23	2.10	0.51
1:A:57:TYR:C	1:A:57:TYR:CD1	2.88	0.51
1:A:96:ALA:O	1:A:165:HIS:HB3	2.11	0.51
1:A:390:GLU:CG	1:A:391:PRO:HD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:OE2	1:A:329:LYS:NZ	2.39	0.50
1:A:7:THR:HG22	1:A:8:PRO:CD	2.38	0.50
1:A:161:LYS:C	1:A:162:LEU:HD12	2.36	0.50
1:A:213:ARG:HB3	1:A:330:GLU:OE1	2.12	0.50
1:A:53:ALA:HA	1:A:105:ILE:HG13	1.93	0.49
1:A:324:PRO:HG3	1:A:343:TYR:OH	2.12	0.49
1:A:372:LEU:O	1:A:376:MET:HG3	2.11	0.49
1:A:261:PHE:HA	1:A:264:VAL:HG12	1.94	0.49
1:A:92:SER:HB2	1:A:111:GLN:OE1	2.12	0.49
1:A:66:ILE:H	1:A:66:ILE:CD1	2.21	0.49
1:A:68:PHE:O	1:A:80:LEU:HD23	2.13	0.49
1:A:277:MET:HE3	1:A:326:LEU:HD21	1.94	0.49
1:A:395:SER:O	1:A:436:LYS:HA	2.14	0.48
1:A:364:MET:HG3	1:A:365:PHE:CE2	2.48	0.48
1:A:88:PHE:HD2	1:A:175:ALA:HB2	1.78	0.48
1:A:291:ALA:HB2	1:A:311:LEU:HB3	1.95	0.48
1:A:130:GLU:HA	1:A:133:ARG:HG3	1.96	0.48
1:A:211:GLU:OE1	1:A:212:PRO:HD2	2.14	0.47
1:A:204:SER:HB3	1:A:335:TYR:CE2	2.49	0.47
1:A:96:ALA:HB1	1:A:169:TRP:CD1	2.50	0.47
1:A:319:MET:HG3	1:A:323:LEU:HD12	1.96	0.47
1:A:28:MET:HE2	1:A:32:LEU:HD11	1.96	0.47
1:A:72:SER:HA	1:A:76:GLY:O	2.14	0.47
1:A:52:ILE:HG22	1:A:105:ILE:CD1	2.43	0.47
1:A:94:ILE:HG21	1:A:106:LEU:HD22	1.96	0.47
1:A:142:VAL:HG22	1:A:261:PHE:CD1	2.50	0.47
1:A:284:CYS:CB	1:A:319:MET:HE2	2.45	0.47
1:A:158:ILE:HG23	1:A:167:LEU:HD12	1.97	0.46
1:A:7:THR:OG1	1:A:10:GLU:HG3	2.14	0.46
1:A:26:LEU:HD23	1:A:151:ALA:HB2	1.97	0.46
1:A:239:LEU:HB3	1:A:249:HIS:NE2	2.30	0.46
1:A:154:LEU:HA	1:A:157:ILE:HB	1.97	0.46
1:A:200:MET:C	1:A:202:LYS:H	2.23	0.46
1:A:246:ALA:O	1:A:249:HIS:HB2	2.16	0.46
1:A:6:MET:O	1:A:10:GLU:HB2	2.16	0.46
1:A:17:LEU:HD13	1:A:124:LEU:HB2	1.98	0.45
1:A:89:ALA:HB2	1:A:175:ALA:HB3	1.98	0.45
1:A:158:ILE:CG2	1:A:167:LEU:HD12	2.47	0.45
1:A:342:VAL:O	1:A:346:SER:HB3	2.16	0.45
1:A:131:GLN:H	1:A:131:GLN:HG3	1.45	0.45
1:A:414:ARG:HH22	1:A:454:ALA:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD23	1:A:101:ILE:HA	1.98	0.45
1:A:388:MET:HE2	1:A:388:MET:HB2	1.93	0.44
1:A:278:LYS:O	1:A:282:VAL:HG23	2.17	0.44
1:A:74:ARG:HD3	1:A:75:ILE:HG12	2.00	0.44
1:A:116:ILE:O	1:A:120:VAL:HG12	2.17	0.44
1:A:299:GLN:NE2	1:A:368:GLN:HB2	2.33	0.44
1:A:448:GLU:O	1:A:451:ILE:HB	2.17	0.44
1:A:401:ILE:HG13	1:A:432:SER:HA	2.00	0.44
1:A:102:TRP:O	1:A:105:ILE:HG22	2.18	0.44
1:A:11:ARG:O	1:A:15:TRP:HD1	2.01	0.43
1:A:116:ILE:HG13	1:A:120:VAL:CG1	2.48	0.43
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.80	0.43
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.84	0.43
1:A:66:ILE:HG23	1:A:345:THR:HG21	2.01	0.43
1:A:93:VAL:HG22	1:A:169:TRP:CZ3	2.53	0.43
1:A:392:PRO:O	1:A:393:TYR:HB2	2.19	0.43
1:A:185:VAL:HG12	1:A:186:VAL:H	1.84	0.43
1:A:66:ILE:CG1	1:A:67:PRO:HD3	2.45	0.42
1:A:73:ASP:O	1:A:74:ARG:C	2.62	0.42
1:A:393:TYR:O	1:A:394:VAL:HG13	2.20	0.42
1:A:30:MET:HE1	1:A:154:LEU:HG	2.00	0.42
1:A:167:LEU:O	1:A:171:ILE:HG13	2.20	0.42
1:A:185:VAL:HG12	1:A:186:VAL:N	2.35	0.42
1:A:409:GLU:H	1:A:409:GLU:CD	2.28	0.42
1:A:72:SER:O	1:A:77:ARG:NH1	2.53	0.42
1:A:77:ARG:N	1:A:79:PRO:HD2	2.34	0.42
1:A:70:LEU:O	1:A:73:ASP:HB2	2.19	0.42
1:A:250:TRP:CE3	1:A:251:LYS:HA	2.54	0.42
1:A:30:MET:SD	1:A:170:MET:HE1	2.60	0.42
1:A:71:LEU:C	1:A:73:ASP:H	2.28	0.42
1:A:284:CYS:HB3	1:A:319:MET:HE2	2.02	0.42
1:A:340:MET:O	1:A:343:TYR:HB3	2.19	0.42
1:A:401:ILE:HG22	1:A:402:PRO:O	2.20	0.42
1:A:239:LEU:HD23	1:A:239:LEU:HA	1.92	0.41
1:A:28:MET:O	1:A:32:LEU:HG	2.20	0.41
1:A:323:LEU:O	1:A:327:ILE:HD12	2.21	0.41
1:A:43:GLN:HB2	1:A:100:SER:HB2	2.03	0.41
1:A:218:ASN:OD1	1:A:343:TYR:HA	2.21	0.41
1:A:284:CYS:SG	1:A:318:LEU:HD23	2.61	0.41
1:A:40:MET:HA	1:A:45:ALA:CB	2.50	0.41
1:A:41:ALA:O	1:A:42:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HD12	1:A:345:THR:HG21	2.02	0.41
1:A:74:ARG:HD3	1:A:75:ILE:CG1	2.50	0.41
1:A:164:LEU:HD12	1:A:164:LEU:HA	1.88	0.41
1:A:4:TYR:CD1	1:A:4:TYR:N	2.88	0.40
1:A:256:THR:HG21	1:A:309:VAL:HG13	2.03	0.40
1:A:449:GLN:HA	1:A:452:ARG:CZ	2.52	0.40
1:A:39:GLY:O	1:A:40:MET:HB2	2.22	0.40
1:A:46:SER:O	1:A:50:ILE:HG12	2.21	0.40
1:A:196:ARG:HE	1:A:196:ARG:HB3	1.39	0.40
1:A:213:ARG:NH1	1:A:330:GLU:HB3	2.35	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	451/453 (100%)	415 (92%)	31 (7%)	5 (1%)	11	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	199	GLY
1	A	42	LEU
1	A	75	ILE
1	A	201	VAL

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	353/354 (100%)	271 (77%)	82 (23%)	1 4

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	4	TYR
1	A	6	MET
1	A	7	THR
1	A	20	VAL
1	A	23	LEU
1	A	24	ARG
1	A	26	LEU
1	A	28	MET
1	A	42	LEU
1	A	43	GLN
1	A	49	LEU
1	A	56	ILE
1	A	57	TYR
1	A	61	GLN
1	A	65	GLN
1	A	66	ILE
1	A	70	LEU
1	A	72	SER
1	A	75	ILE
1	A	78	LYS
1	A	85	LEU
1	A	92	SER
1	A	93	VAL
1	A	94	ILE
1	A	98	SER
1	A	100	SER
1	A	101	ILE
1	A	104	ILE
1	A	106	LEU
1	A	108	ARG
1	A	120	VAL
1	A	121	MET
1	A	124	LEU

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Mol	Chain	Res	Type
1	A	125	SER
1	A	131	GLN
1	A	143	SER
1	A	150	ILE
1	A	152	MET
1	A	154	LEU
1	A	159	THR
1	A	160	HIS
1	A	161	LYS
1	A	162	LEU
1	A	167	LEU
1	A	181	LEU
1	A	215	LEU
1	A	216	LYS
1	A	222	MET
1	A	226	MET
1	A	231	THR
1	A	233	VAL
1	A	235	LEU
1	A	244	PHE
1	A	254	LEU
1	A	256	THR
1	A	257	MET
1	A	265	VAL
1	A	268	ILE
1	A	272	GLU
1	A	276	LYS
1	A	285	VAL
1	A	287	LEU
1	A	293	ILE
1	A	297	ASN
1	A	299	GLN
1	A	300	THR
1	A	302	PHE
1	A	307	VAL
1	A	323	LEU
1	A	325	SER
1	A	327	ILE
1	A	329	LYS
1	A	336	LYS
1	A	345	THR
1	A	346	SER

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Mol	Chain	Res	Type
1	A	349	LEU
1	A	351	VAL
1	A	370	VAL
1	A	388	MET
1	A	389	LYS
1	A	441	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	301	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	453/453 (100%)	0.24	21 (4%)	37 21	33, 54, 138, 222	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	GLU	6.7
1	A	244	PHE	4.3
1	A	201	VAL	4.1
1	A	186	VAL	3.9
1	A	402	PRO	3.4
1	A	409	GLU	3.4
1	A	187	PRO	3.1
1	A	301	GLN	2.6
1	A	193	VAL	2.6
1	A	65	GLN	2.5
1	A	194	LEU	2.5
1	A	188	ASN	2.4
1	A	348	PHE	2.4
1	A	200	MET	2.3
1	A	416	LEU	2.2
1	A	158	ILE	2.2
1	A	414	ARG	2.2
1	A	40	MET	2.1
1	A	192	HIS	2.1
1	A	205	PHE	2.1
1	A	299	GLN	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.