



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:11 am BST

PDB ID : 4JA3  
Title : Partially occluded inward open conformation of the xylose transporter XylE from *E. coli*  
Authors : Quistgaard, E.M.; Low, C.; Moberg, P.; Tresaugues, L.; Nordlund, P.  
Deposited on : 2013-02-18  
Resolution : 3.80 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](mailto: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.

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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	:	2.11
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)	:	2.11

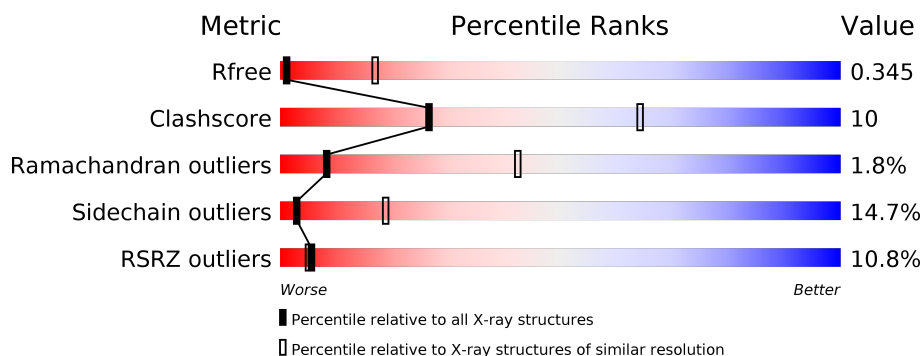
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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  $\geq 3$ , 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	485	<div> <div>7%</div> <div>59%</div> <div>25%</div> <div>•</div> <div>12%</div> </div>
1	B	485	<div> <div>12%</div> <div>64%</div> <div>23%</div> <div>•</div> <div>9%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6626 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 D-xylose-proton symporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3262	2156	517	566	23			
1	B	439	Total	C	N	O	S	0	0	0
			3359	2220	533	583	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P0AGF4
B	1	GLY	-	EXPRESSION TAG	UNP P0AGF4

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		

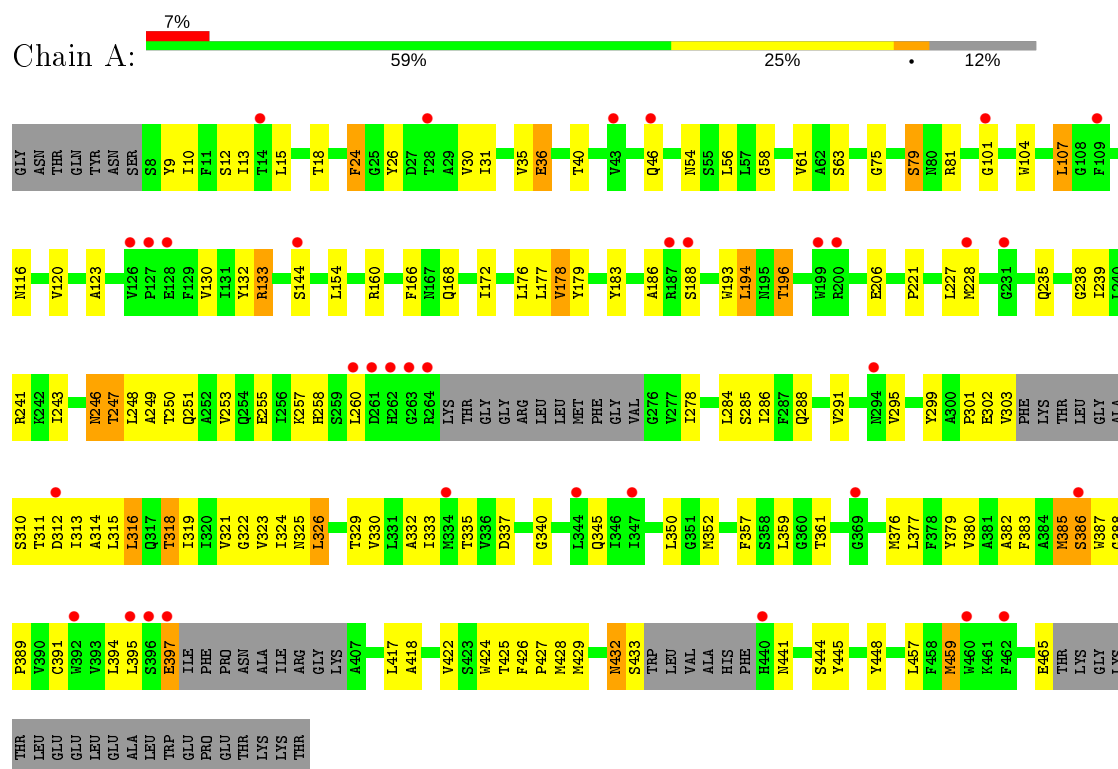
- Molecule 3 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Lu	0	0
			2	2		
3	A	2	Total	Lu	0	0
			2	2		

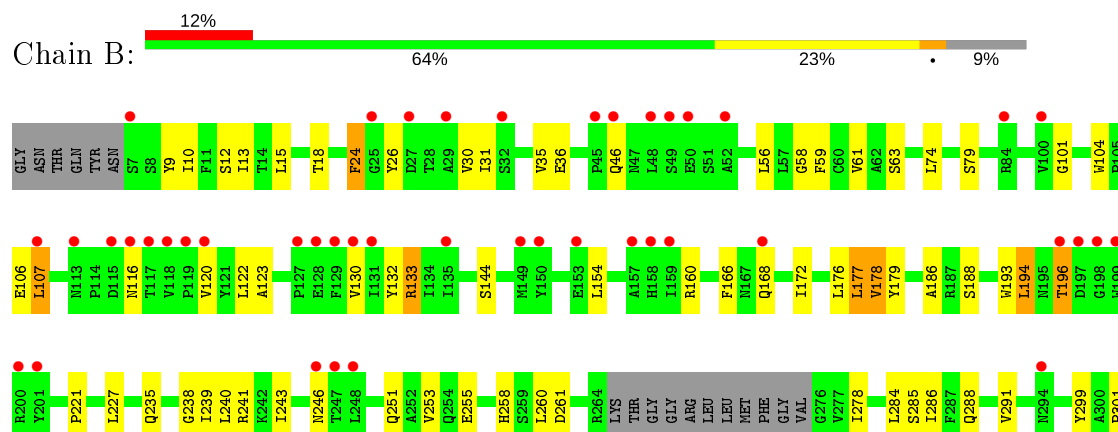
### 3 Residue-property plots [i](#)

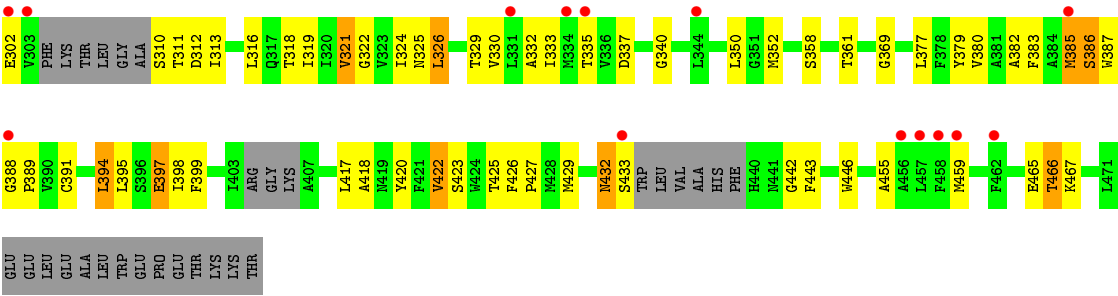
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: D-xylose-proton symporter



- Molecule 1: D-xylose-proton symporter





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	246.88Å 74.38Å 131.11Å 90.00° 117.71° 90.00°	Depositor
Resolution (Å)	25.26 – 3.80 48.49 – 3.80	Depositor EDS
% Data completeness (in resolution range)	82.3 (25.26-3.80) 82.4 (48.49-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.285 , 0.315 0.314 , 0.345	Depositor DCC
$R_{free}$ test set	1348 reflections (7.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	154.0	Xtriage
Anisotropy	0.915	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 148.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	6626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	232.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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

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	0.43	0/3343	0.62	1/4547 (0.0%)
1	B	0.45	0/3442	0.67	1/4681 (0.0%)
All	All	0.44	0/6785	0.65	2/9228 (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	B	432	ASN	C-N-CA	5.29	134.92	121.70
1	A	432	ASN	C-N-CA	5.07	134.38	121.70

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	3262	0	3303	77	0
1	B	3359	0	3411	61	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	6626	0	6714	138	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 10.

All (138) 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:332:ALA:HB1	1:B:389:PRO:HG3	1.32	1.10
1:A:332:ALA:HB1	1:A:389:PRO:HG3	1.33	1.08
1:A:249:ALA:O	1:A:253:VAL:HG23	1.71	0.90
1:A:58:GLY:HA2	1:A:427:PRO:HG2	1.51	0.89
1:A:183:TYR:HA	1:A:315:LEU:HD13	1.56	0.85
1:A:30:VAL:CG1	1:A:178:VAL:HG11	2.08	0.84
1:B:30:VAL:CG1	1:B:178:VAL:HG11	2.09	0.82
1:A:10:ILE:HB	1:A:243:ILE:HG12	1.62	0.81
1:B:10:ILE:HB	1:B:243:ILE:HG12	1.64	0.80
1:A:332:ALA:CB	1:A:389:PRO:HG3	2.12	0.79
1:A:58:GLY:CA	1:A:427:PRO:HG2	2.13	0.79
1:B:332:ALA:CB	1:B:389:PRO:HG3	2.13	0.74
1:A:30:VAL:HG12	1:A:178:VAL:HG11	1.68	0.74
1:B:30:VAL:HG12	1:B:178:VAL:HG11	1.67	0.73
1:A:284:LEU:O	1:A:288:GLN:HG3	1.88	0.73
1:B:284:LEU:O	1:B:288:GLN:HG3	1.89	0.71
1:A:179:TYR:HB3	1:A:319:ILE:HG12	1.73	0.71
1:A:176:LEU:HD21	1:A:322:GLY:O	1.93	0.68
1:A:30:VAL:HG13	1:A:178:VAL:HG11	1.75	0.67
1:A:321:VAL:HG13	1:A:380:VAL:HG21	1.76	0.67
1:B:394:LEU:HA	1:B:398:ILE:HD13	1.78	0.66
1:B:30:VAL:HG13	1:B:178:VAL:HG11	1.77	0.65
1:A:352:MET:HB2	1:A:379:TYR:CD2	2.32	0.64
1:B:288:GLN:HG2	1:B:387:TRP:HE1	1.63	0.64
1:A:324:ILE:HG13	1:A:377:LEU:HD22	1.79	0.63
1:A:288:GLN:HG2	1:A:387:TRP:HE1	1.63	0.63
1:B:352:MET:HB2	1:B:379:TYR:CD2	2.34	0.62
1:B:9:TYR:HB3	1:B:243:ILE:HD13	1.82	0.62
1:A:228:MET:CE	1:A:257:LYS:HG2	2.30	0.61
1:A:9:TYR:HB3	1:A:243:ILE:HD13	1.81	0.61
1:B:258:HIS:HA	1:B:261:ASP:HB3	1.83	0.61
1:A:172:ILE:HG22	1:A:326:LEU:HD12	1.83	0.60
1:A:24:PHE:HE1	1:A:144:SER:HB2	1.66	0.60
1:B:24:PHE:HE1	1:B:144:SER:HB2	1.66	0.59
1:A:176:LEU:HD21	1:A:322:GLY:C	2.23	0.59
1:B:172:ILE:HG22	1:B:326:LEU:HD12	1.84	0.59
1:B:324:ILE:HG13	1:B:377:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:SER:HA	1:B:288:GLN:CD	2.24	0.58
1:A:310:SER:HB3	1:A:313:ILE:HB	1.83	0.58
1:B:321:VAL:HG23	1:B:377:LEU:HD23	1.85	0.58
1:A:285:SER:HA	1:A:288:GLN:CD	2.23	0.58
1:A:18:THR:HG21	1:A:166:PHE:HD1	1.69	0.57
1:A:30:VAL:HG12	1:A:178:VAL:CG1	2.34	0.57
1:A:61:VAL:HG21	1:A:299:TYR:OH	2.04	0.57
1:A:345:GLN:HB2	1:A:459:MET:SD	2.44	0.57
1:B:18:THR:HG21	1:B:166:PHE:HD1	1.70	0.57
1:A:101:GLY:HA3	1:A:132:TYR:CD2	2.40	0.57
1:B:101:GLY:HA3	1:B:132:TYR:CD2	2.40	0.56
1:B:30:VAL:HG12	1:B:178:VAL:CG1	2.34	0.56
1:A:352:MET:HE3	1:A:383:PHE:HB2	1.88	0.56
1:A:303:VAL:HG11	1:A:445:TYR:OH	2.06	0.55
1:B:352:MET:HE3	1:B:383:PHE:HB2	1.89	0.54
1:B:58:GLY:HA2	1:B:427:PRO:HG2	1.89	0.54
1:B:394:LEU:O	1:B:398:ILE:HB	2.07	0.54
1:A:160:ARG:HH21	1:A:397:GLU:HB3	1.73	0.54
1:A:238:GLY:HA2	1:A:241:ARG:HE	1.74	0.53
1:B:61:VAL:HG21	1:B:299:TYR:OH	2.09	0.53
1:B:193:TRP:HA	1:B:196:THR:HG22	1.89	0.52
1:A:193:TRP:HA	1:A:196:THR:HG22	1.90	0.52
1:A:301:PRO:HG3	1:A:318:THR:HG21	1.90	0.52
1:B:221:PRO:HB2	1:B:239:ILE:HD13	1.92	0.51
1:B:466:THR:O	1:B:467:LYS:HB3	2.10	0.51
1:A:313:ILE:O	1:A:316:LEU:HB3	2.10	0.51
1:A:228:MET:HE1	1:A:257:LYS:CG	2.41	0.50
1:A:26:TYR:CZ	1:A:178:VAL:HG13	2.47	0.50
1:A:321:VAL:CG1	1:A:380:VAL:HG21	2.41	0.50
1:B:238:GLY:HA2	1:B:241:ARG:HE	1.77	0.50
1:B:160:ARG:HH21	1:B:397:GLU:HB3	1.76	0.50
1:B:455:ALA:O	1:B:459:MET:HG3	2.11	0.50
1:A:228:MET:HE1	1:A:257:LYS:HG2	1.92	0.50
1:A:221:PRO:HB2	1:A:239:ILE:HD13	1.92	0.50
1:B:176:LEU:HD21	1:B:322:GLY:O	2.12	0.50
1:B:382:ALA:O	1:B:386:SER:HB3	2.12	0.49
1:B:288:GLN:HG2	1:B:387:TRP:NE1	2.26	0.49
1:A:9:TYR:CE2	1:A:13:ILE:HD11	2.48	0.49
1:B:46:GLN:HG2	1:B:123:ALA:HB1	1.95	0.49
1:A:330:VAL:O	1:A:333:ILE:HG12	2.13	0.49
1:B:332:ALA:HB1	1:B:389:PRO:CG	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ALA:HB1	1:A:389:PRO:CG	2.23	0.48
1:A:288:GLN:HG2	1:A:387:TRP:NE1	2.26	0.48
1:A:286:ILE:HG22	1:A:418:ALA:HB2	1.95	0.48
1:B:361:THR:HG23	1:B:446:TRP:HE1	1.78	0.48
1:B:9:TYR:CE2	1:B:13:ILE:HD11	2.48	0.48
1:B:286:ILE:HG22	1:B:418:ALA:HB2	1.95	0.48
1:A:179:TYR:HB3	1:A:319:ILE:CG1	2.43	0.48
1:B:26:TYR:CZ	1:B:178:VAL:HG13	2.48	0.48
1:A:382:ALA:O	1:A:386:SER:HB3	2.13	0.48
1:B:330:VAL:O	1:B:333:ILE:HG12	2.13	0.48
1:A:63:SER:HB2	1:A:130:VAL:HG13	1.96	0.48
1:B:133:ARG:HA	1:B:133:ARG:HD2	1.53	0.47
1:B:255:GLU:HA	1:B:258:HIS:CE1	2.50	0.47
1:A:46:GLN:HG2	1:A:123:ALA:HB1	1.96	0.47
1:A:75:GLY:O	1:A:79:SER:HB2	2.14	0.47
1:B:426:PHE:HB3	1:B:427:PRO:HD3	1.96	0.47
1:A:314:ALA:O	1:A:318:THR:HG23	2.15	0.46
1:A:310:SER:O	1:A:314:ALA:N	2.38	0.46
1:A:246:ASN:O	1:A:250:THR:OG1	2.31	0.46
1:A:183:TYR:HA	1:A:315:LEU:CD1	2.35	0.46
1:A:295:VAL:HG21	1:A:448:TYR:OH	2.16	0.46
1:B:63:SER:HB2	1:B:130:VAL:HG13	1.97	0.46
1:A:345:GLN:CB	1:A:459:MET:SD	3.03	0.46
1:A:299:TYR:CD2	1:A:426:PHE:CD2	3.05	0.45
1:A:422:VAL:HA	1:A:425:THR:HG22	1.99	0.44
1:B:301:PRO:HG3	1:B:318:THR:HG21	1.99	0.44
1:A:359:LEU:HD22	1:A:376:MET:HG2	1.99	0.44
1:A:357:PHE:O	1:A:361:THR:HG23	2.17	0.44
1:B:321:VAL:HG22	1:B:380:VAL:HG21	1.99	0.44
1:A:352:MET:HB2	1:A:379:TYR:CE2	2.53	0.44
1:A:172:ILE:HD13	1:A:329:THR:HG21	1.98	0.44
1:A:288:GLN:CG	1:A:387:TRP:HE1	2.30	0.43
1:B:255:GLU:HA	1:B:258:HIS:HE1	1.81	0.43
1:B:179:TYR:HB3	1:B:319:ILE:HG12	2.00	0.43
1:B:106:GLU:HB3	1:B:122:LEU:HD21	1.99	0.43
1:B:172:ILE:HD13	1:B:329:THR:HG21	2.01	0.43
1:B:422:VAL:HA	1:B:425:THR:HG22	2.01	0.43
1:A:104:TRP:O	1:A:107:LEU:HB2	2.19	0.43
1:A:36:GLU:O	1:A:40:THR:HG23	2.19	0.43
1:B:176:LEU:HD21	1:B:322:GLY:C	2.39	0.43
1:A:247:THR:OG1	1:A:248:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ALA:HB2	1:A:385:MET:HA	2.01	0.43
1:B:186:ALA:HA	1:B:194:LEU:HD11	2.00	0.42
1:B:288:GLN:CG	1:B:387:TRP:HE1	2.31	0.42
1:A:186:ALA:HA	1:A:194:LEU:HD11	2.00	0.42
1:B:104:TRP:O	1:B:107:LEU:HB2	2.20	0.42
1:B:310:SER:HB2	1:B:313:ILE:HB	2.01	0.42
1:B:26:TYR:HE1	1:B:177:LEU:HD22	1.86	0.41
1:B:332:ALA:HB2	1:B:385:MET:HA	2.01	0.41
1:A:299:TYR:CE2	1:A:426:PHE:CD2	3.08	0.41
1:A:424:TRP:O	1:A:427:PRO:HD2	2.20	0.41
1:A:54:ASN:HB3	1:A:428:MET:HA	2.02	0.41
1:B:352:MET:HB2	1:B:379:TYR:CE2	2.56	0.41
1:A:133:ARG:HD2	1:A:133:ARG:HA	1.55	0.41
1:A:176:LEU:HD11	1:A:323:VAL:N	2.36	0.41
1:A:9:TYR:O	1:A:13:ILE:HG13	2.21	0.41
1:A:352:MET:HE1	1:A:383:PHE:HD2	1.85	0.41
1:B:59:PHE:HD1	1:B:420:TYR:HH	1.67	0.40
1:A:26:TYR:CE2	1:A:206:GLU:HB2	2.56	0.40
1:B:24:PHE:CE1	1:B:144:SER:HB2	2.52	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	416/485 (86%)	387 (93%)	22 (5%)	7 (2%)	9	43
1	B	429/485 (88%)	398 (93%)	23 (5%)	8 (2%)	8	42
All	All	845/970 (87%)	785 (93%)	45 (5%)	15 (2%)	8	42

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	LEU
1	B	107	LEU
1	A	116	ASN
1	B	116	ASN
1	A	247	THR
1	B	35	VAL
1	A	35	VAL
1	A	120	VAL
1	B	120	VAL
1	A	340	GLY
1	B	388	GLY
1	A	388	GLY
1	B	340	GLY
1	B	369	GLY
1	B	442	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	342/390 (88%)	292 (85%)	50 (15%)	3	19
1	B	353/390 (90%)	301 (85%)	52 (15%)	3	19
All	All	695/780 (89%)	593 (85%)	102 (15%)	3	19

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	15	LEU
1	A	24	PHE
1	A	31	ILE
1	A	36	GLU
1	A	56	LEU
1	A	79	SER
1	A	81	ARG
1	A	133	ARG

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Mol	Chain	Res	Type
1	A	154	LEU
1	A	168	GLN
1	A	177	LEU
1	A	178	VAL
1	A	188	SER
1	A	194	LEU
1	A	196	THR
1	A	227	LEU
1	A	235	GLN
1	A	246	ASN
1	A	251	GLN
1	A	255	GLU
1	A	258	HIS
1	A	260	LEU
1	A	278	ILE
1	A	291	VAL
1	A	302	GLU
1	A	311	THR
1	A	312	ASP
1	A	316	LEU
1	A	318	THR
1	A	325	ASN
1	A	326	LEU
1	A	335	THR
1	A	337	ASP
1	A	350	LEU
1	A	385	MET
1	A	386	SER
1	A	391	CYS
1	A	394	LEU
1	A	395	LEU
1	A	397	GLU
1	A	417	LEU
1	A	429	MET
1	A	432	ASN
1	A	433	SER
1	A	441	ASN
1	A	444	SER
1	A	457	LEU
1	A	459	MET
1	A	465	GLU
1	B	12	SER

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Mol	Chain	Res	Type
1	B	15	LEU
1	B	24	PHE
1	B	31	ILE
1	B	36	GLU
1	B	56	LEU
1	B	74	LEU
1	B	79	SER
1	B	133	ARG
1	B	154	LEU
1	B	168	GLN
1	B	177	LEU
1	B	178	VAL
1	B	188	SER
1	B	194	LEU
1	B	196	THR
1	B	227	LEU
1	B	235	GLN
1	B	240	LEU
1	B	246	ASN
1	B	251	GLN
1	B	253	VAL
1	B	260	LEU
1	B	278	ILE
1	B	291	VAL
1	B	302	GLU
1	B	311	THR
1	B	312	ASP
1	B	316	LEU
1	B	321	VAL
1	B	325	ASN
1	B	326	LEU
1	B	335	THR
1	B	337	ASP
1	B	350	LEU
1	B	358	SER
1	B	385	MET
1	B	386	SER
1	B	391	CYS
1	B	394	LEU
1	B	395	LEU
1	B	397	GLU
1	B	399	PHE

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Mol	Chain	Res	Type
1	B	417	LEU
1	B	422	VAL
1	B	423	SER
1	B	429	MET
1	B	432	ASN
1	B	433	SER
1	B	443	PHE
1	B	465	GLU
1	B	466	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	262	HIS
1	A	325	ASN
1	B	233	GLN
1	B	325	ASN
1	B	366	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 ⓘ

Of 5 ligands modelled in this entry, 5 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

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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	426/485 (87%)	0.36	35 (8%)	11 9	166, 229, 268, 275	0
1	B	439/485 (90%)	0.47	58 (13%)	3 3	170, 235, 271, 284	0
All	All	865/970 (89%)	0.41	93 (10%)	5 5	166, 231, 270, 284	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	ARG	8.2
1	B	335	THR	8.1
1	B	197	ASP	6.2
1	B	201	TYR	5.8
1	B	331	LEU	5.4
1	A	187	ARG	5.2
1	B	158	HIS	5.0
1	B	115	ASP	4.7
1	A	127	PRO	4.3
1	A	263	GLY	4.3
1	B	48	LEU	4.2
1	A	396	SER	4.2
1	A	144	SER	4.1
1	B	118	VAL	4.0
1	B	159	ILE	4.0
1	A	199	TRP	3.9
1	A	312	ASP	3.9
1	A	46	GLN	3.9
1	A	228	MET	3.8
1	B	196	THR	3.8
1	B	153	GLU	3.7
1	B	116	ASN	3.6
1	B	458	PHE	3.6
1	B	334	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	247	THR	3.6
1	B	294	ASN	3.5
1	A	261	ASP	3.5
1	A	397	GLU	3.4
1	A	128	GLU	3.4
1	B	459	MET	3.4
1	A	188	SER	3.3
1	B	119	PRO	3.3
1	B	150	TYR	3.3
1	B	29	ALA	3.2
1	B	385	MET	3.2
1	B	46	GLN	3.2
1	A	200	ARG	3.2
1	B	84	ARG	3.1
1	A	14	THR	2.9
1	B	131	ILE	2.9
1	A	260	LEU	2.9
1	B	457	LEU	2.8
1	A	231	GLY	2.8
1	A	386	SER	2.8
1	B	433	SER	2.8
1	B	344	LEU	2.7
1	A	294	ASN	2.7
1	A	395	LEU	2.7
1	B	49	SER	2.7
1	B	157	ALA	2.7
1	B	120	VAL	2.7
1	A	344	LEU	2.7
1	B	25	GLY	2.7
1	B	113	ASN	2.6
1	A	109	PHE	2.6
1	A	440	HIS	2.6
1	B	198	GLY	2.6
1	A	460	TRP	2.5
1	A	126	VAL	2.5
1	B	107	LEU	2.5
1	B	462	PHE	2.5
1	B	303	VAL	2.5
1	A	43	VAL	2.5
1	B	127	PRO	2.5
1	A	334	MET	2.4
1	B	27	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	129	PHE	2.4
1	B	7	SER	2.4
1	A	262	HIS	2.4
1	B	52	ALA	2.4
1	B	200	ARG	2.4
1	A	347	ILE	2.3
1	B	45	PRO	2.3
1	B	128	GLU	2.3
1	B	248	LEU	2.3
1	B	149	MET	2.3
1	B	246	ASN	2.2
1	B	388	GLY	2.2
1	B	130	VAL	2.2
1	B	135	ILE	2.2
1	A	101	GLY	2.1
1	A	392	TRP	2.1
1	A	369	GLY	2.1
1	B	117	THR	2.1
1	B	302	GLU	2.1
1	A	28	THR	2.1
1	B	168	GLN	2.1
1	B	50	GLU	2.1
1	B	199	TRP	2.1
1	B	100	VAL	2.1
1	B	456	ALA	2.1
1	A	462	PHE	2.1
1	B	32	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	LU	B	502	1/1	0.74	0.11	300,300,300,300	0
3	LU	A	502	1/1	0.92	0.13	300,300,300,300	0
2	CD	A	501	1/1	0.95	0.11	300,300,300,300	0
3	LU	B	501	1/1	0.97	0.19	300,300,300,300	0
3	LU	A	503	1/1	0.98	0.25	295,295,295,295	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.