



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:09 am BST

PDB ID : 4JA4
Title : 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 : 4.20 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 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

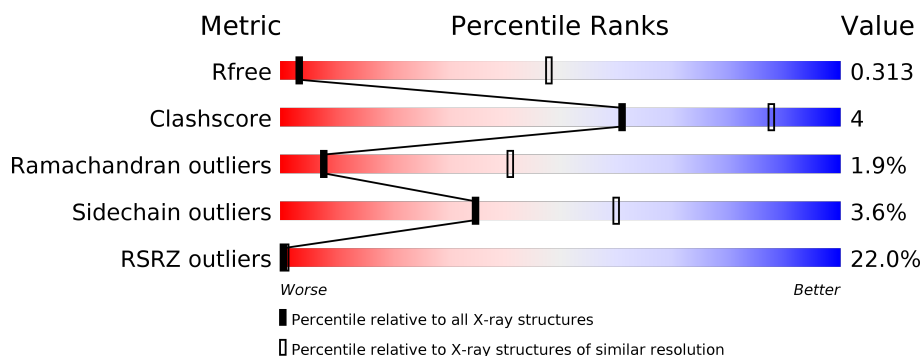
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 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>20%</div> <div>75%</div> <div>15%</div> <div>• 9%</div> </div>
1	B	485	<div> <div>18%</div> <div>76%</div> <div>13%</div> <div>• 9%</div> </div>
1	C	485	<div> <div>22%</div> <div>76%</div> <div>12%</div> <div>• 10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10130 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	442	Total	C	N	O	S	0	0	0
			3401	2257	533	587	24			
1	B	439	Total	C	N	O	S	0	0	0
			3379	2242	530	583	24			
1	C	436	Total	C	N	O	S	0	0	0
			3349	2225	524	576	24			

There are 3 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
C	1	GLY	-	EXPRESSION TAG	UNP P0AGF4

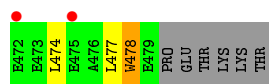
- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

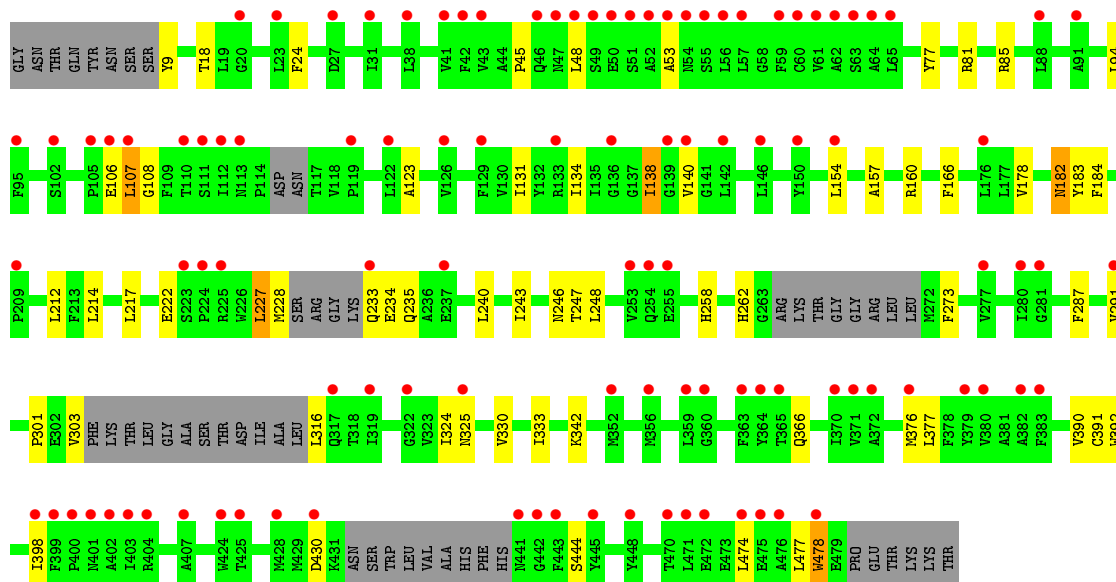
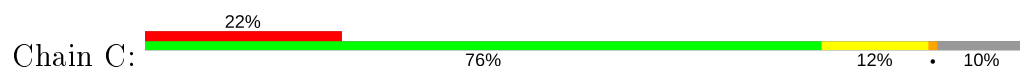
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

- [illegible]

- Chain B:
-
- 18% 76% 13% 9%
- GLY ASN THR GLN TYR ASN SER SER Y9 V16 A17 T18 F24 F42 V43 A44 P45 Q46 F50 S51 A52 A53 N54 S55 L56 L57 Y77 R81 R84 R85 L88 L94 E106 L107 G108 F109 T110 S111 I112 M113 P114 D115 N116 THR VAL P119 A123 T124 I134 I138 G139 V140 Y150 Y154 A157 R160 F166 V178 M182 Y183 F184 I185 A186 R187 S188 G189 H193 Y201 L212 L213 L214 L217 V220 P221 E222 S223 P224 R225 L226 W227 M228 SER ARG GLY LYS Q233 Q234 Q235 E236 E237 N246 T247 I249 Q254 H258 H262 G263 LYS THR GLY GLY ARG LEU M272 F273 F287 V291 V303 PHE LYS THR LEU GLY ALA SER THR ASP ILE ALA LEU L316 Q317 Q317 V321 I324 T335 V336 D337 K338 F339 G340 R341 K342 P343 L344 Q345 Y445 Y446 I447 Y448 W460 T474 G360 T361 A362 F363 Q366 G369 I370 V371 A372 M376 L377 F378 V379 V380 A381 A382 M385 S386 S387 V390 C391 W392 I398 F399 P400 N401 A402 I403 R404 G405 D430 K431 N432 S433 W434 LEU VAL ALA HIS PHE HIS N441 G442 F443 F444 S444 Y445 Y446 I447 Y448 W460 T474



● Molecule 1: D-xylose-proton symporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	125.82Å 125.82Å 380.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.18 – 4.20 71.68 – 4.20	Depositor EDS
% Data completeness (in resolution range)	72.2 (41.18-4.20) 72.4 (71.68-4.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 4.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.288 , 0.318 0.288 , 0.313	Depositor DCC
R_{free} test set	1374 reflections (7.66%)	wwPDB-VP
Wilson B-factor (Å ²)	161.4	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 139.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.085 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.61	EDS
Total number of atoms	10130	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.22	0/3488	0.37	0/4745
1	B	0.22	0/3465	0.37	0/4710
1	C	0.22	0/3433	0.37	0/4667
All	All	0.22	0/10386	0.37	0/14122

There are no bond length outliers.

There are no bond angle outliers.

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	3401	0	3445	36	0
1	B	3379	0	3418	30	0
1	C	3349	0	3402	26	0
2	A	1	0	0	0	0
All	All	10130	0	10265	91	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 (91) 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:C:258:HIS:CE1	1:C:262:HIS:NE2	2.57	0.72
1:B:258:HIS:CE1	1:B:262:HIS:NE2	2.59	0.70
1:A:258:HIS:CE1	1:A:262:HIS:NE2	2.62	0.66
1:B:227:LEU:N	1:B:228:MET:HA	2.13	0.64
1:A:227:LEU:N	1:A:228:MET:HA	2.13	0.62
1:C:227:LEU:N	1:C:228:MET:HA	2.13	0.62
1:C:178:VAL:O	1:C:182:ASN:ND2	2.33	0.60
1:A:178:VAL:O	1:A:182:ASN:ND2	2.34	0.60
1:C:85:ARG:HD2	1:C:222:GLU:HG3	1.84	0.60
1:B:85:ARG:HD2	1:B:222:GLU:HG3	1.84	0.59
1:A:85:ARG:HD2	1:A:222:GLU:HG3	1.83	0.59
1:B:227:LEU:H	1:B:228:MET:HA	1.68	0.59
1:C:18:THR:HG21	1:C:166:PHE:HD1	1.68	0.58
1:C:94:LEU:HD13	1:C:138:ILE:HG23	1.85	0.58
1:B:273:PHE:HE1	1:B:478:TRP:HB2	1.69	0.57
1:C:227:LEU:H	1:C:228:MET:HA	1.69	0.57
1:A:227:LEU:H	1:A:228:MET:HA	1.68	0.56
1:C:430:ASP:HB2	1:C:444:SER:HB3	1.87	0.56
1:C:390:VAL:O	1:C:392:TRP:N	2.38	0.56
1:A:390:VAL:O	1:A:392:TRP:N	2.39	0.56
1:B:94:LEU:HD13	1:B:138:ILE:HG23	1.88	0.55
1:C:273:PHE:HE1	1:C:478:TRP:HB2	1.71	0.55
1:B:390:VAL:O	1:B:392:TRP:N	2.39	0.55
1:B:430:ASP:HB2	1:B:444:SER:HB3	1.88	0.55
1:A:430:ASP:HB2	1:A:444:SER:HB3	1.89	0.55
1:B:18:THR:HG21	1:B:166:PHE:HD1	1.72	0.54
1:A:317:GLN:O	1:A:321:VAL:HG23	2.09	0.53
1:A:273:PHE:HE1	1:A:478:TRP:HB2	1.72	0.53
1:B:178:VAL:O	1:B:182:ASN:ND2	2.36	0.53
1:C:106:GLU:O	1:C:108:GLY:N	2.43	0.52
1:A:94:LEU:HD13	1:A:138:ILE:HG23	1.91	0.52
1:B:214:LEU:HA	1:B:217:LEU:HD12	1.90	0.52
1:A:106:GLU:O	1:A:108:GLY:N	2.43	0.52
1:A:18:THR:HG21	1:A:166:PHE:HD1	1.75	0.51
1:B:106:GLU:O	1:B:108:GLY:N	2.43	0.51
1:A:433:SER:O	1:A:434:TRP:HB2	2.11	0.51
1:A:324:ILE:HG13	1:A:377:LEU:HD22	1.93	0.50
1:B:433:SER:O	1:B:434:TRP:HB2	2.11	0.49
1:C:474:LEU:HA	1:C:477:LEU:HD13	1.95	0.49
1:B:157:ALA:HA	1:B:160:ARG:HE	1.79	0.48
1:C:214:LEU:HA	1:C:217:LEU:HD12	1.94	0.48
1:B:431:LYS:HA	1:B:432:ASN:HA	1.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLN:O	1:B:235:GLN:N	2.47	0.48
1:A:431:LYS:HA	1:A:432:ASN:HA	1.50	0.47
1:C:233:GLN:O	1:C:235:GLN:N	2.47	0.47
1:A:240:LEU:HA	1:A:243:ILE:HD12	1.96	0.47
1:B:324:ILE:HG13	1:B:377:LEU:HD22	1.96	0.47
1:A:233:GLN:O	1:A:235:GLN:N	2.47	0.46
1:A:157:ALA:HA	1:A:160:ARG:HE	1.81	0.46
1:C:324:ILE:HG13	1:C:377:LEU:HD22	1.97	0.45
1:C:157:ALA:HA	1:C:160:ARG:HE	1.82	0.45
1:B:321:VAL:HG13	1:B:380:VAL:HG21	1.99	0.45
1:B:223:SER:HA	1:B:224:PRO:HD3	1.84	0.44
1:B:115:ASP:OD2	1:B:116:ASN:ND2	2.50	0.44
1:A:110:THR:HG1	1:A:125:TYR:HH	1.64	0.44
1:A:474:LEU:HA	1:A:477:LEU:HD13	1.98	0.44
1:A:214:LEU:HA	1:A:217:LEU:HD12	2.00	0.44
1:B:474:LEU:HA	1:B:477:LEU:HD13	2.00	0.43
1:A:330:VAL:O	1:A:333:ILE:HG12	2.19	0.43
1:C:240:LEU:HA	1:C:243:ILE:HD12	2.01	0.43
1:B:287:PHE:O	1:B:291:VAL:HG23	2.19	0.43
1:A:287:PHE:O	1:A:291:VAL:HG23	2.19	0.42
1:B:246:ASN:O	1:B:248:LEU:N	2.53	0.42
1:B:77:TYR:CZ	1:B:81:ARG:HD2	2.54	0.42
1:C:246:ASN:O	1:C:248:LEU:N	2.52	0.42
1:C:77:TYR:CZ	1:C:81:ARG:HD2	2.54	0.42
1:C:24:PHE:CD1	1:C:140:VAL:HG13	2.54	0.42
1:C:287:PHE:O	1:C:291:VAL:HG23	2.20	0.42
1:C:330:VAL:O	1:C:333:ILE:HG12	2.19	0.42
1:A:115:ASP:OD2	1:A:116:ASN:ND2	2.52	0.42
1:A:246:ASN:O	1:A:248:LEU:N	2.53	0.42
1:B:106:GLU:HG2	1:B:107:LEU:N	2.34	0.42
1:A:223:SER:HA	1:A:224:PRO:HD3	1.84	0.42
1:C:45:PRO:HG2	1:C:123:ALA:HB2	2.00	0.42
1:B:45:PRO:HG2	1:B:123:ALA:HB2	2.02	0.41
1:A:106:GLU:HG2	1:A:107:LEU:N	2.35	0.41
1:A:24:PHE:CD1	1:A:140:VAL:HG13	2.55	0.41
1:B:24:PHE:CD1	1:B:140:VAL:HG13	2.54	0.41
1:C:106:GLU:HG2	1:C:107:LEU:N	2.35	0.41
1:A:463:VAL:HA	1:A:464:PRO:HD3	1.93	0.41
1:C:48:LEU:H	1:C:53:ALA:HB2	1.85	0.41
1:B:342:LYS:HB3	1:B:343:PRO:HD3	2.02	0.41
1:A:45:PRO:HG2	1:A:123:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:CZ	1:A:81:ARG:HD2	2.56	0.41
1:A:407:ALA:HA	1:A:410:ILE:HD12	2.02	0.41
1:A:258:HIS:CE1	1:B:258:HIS:CD2	3.09	0.41
1:A:131:ILE:O	1:A:134:ILE:HG22	2.22	0.40
1:A:115:ASP:HB3	1:A:116:ASN:H	1.75	0.40
1:A:470:THR:HG22	1:A:473:GLU:HB2	2.04	0.40
1:B:131:ILE:O	1:B:134:ILE:HG22	2.21	0.40
1:C:131:ILE:O	1:C:134:ILE:HG22	2.21	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	432/485 (89%)	399 (92%)	24 (6%)	9 (2%)	7	39
1	B	427/485 (88%)	393 (92%)	26 (6%)	8 (2%)	8	41
1	C	424/485 (87%)	394 (93%)	23 (5%)	7 (2%)	9	44
All	All	1283/1455 (88%)	1186 (92%)	73 (6%)	24 (2%)	8	41

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	LEU
1	A	117	THR
1	A	391	CYS
1	B	107	LEU
1	B	391	CYS
1	C	107	LEU
1	C	391	CYS
1	A	227	LEU
1	B	227	LEU

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Mol	Chain	Res	Type
1	B	247	THR
1	C	227	LEU
1	A	234	GLU
1	A	247	THR
1	A	342	LYS
1	B	234	GLU
1	B	342	LYS
1	C	234	GLU
1	C	247	THR
1	C	342	LYS
1	A	366	GLN
1	B	366	GLN
1	B	433	SER
1	C	366	GLN
1	A	433	SER

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	355/390 (91%)	344 (97%)	11 (3%)	40	62
1	B	352/390 (90%)	339 (96%)	13 (4%)	34	59
1	C	349/390 (90%)	335 (96%)	14 (4%)	31	57
All	All	1056/1170 (90%)	1018 (96%)	38 (4%)	35	60

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	138	ILE
1	A	154	LEU
1	A	182	ASN
1	A	183	TYR
1	A	184	PHE
1	A	212	LEU

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Mol	Chain	Res	Type
1	A	316	LEU
1	A	376	MET
1	A	398	ILE
1	A	478	TRP
1	B	9	TYR
1	B	138	ILE
1	B	154	LEU
1	B	182	ASN
1	B	183	TYR
1	B	184	PHE
1	B	212	LEU
1	B	316	LEU
1	B	337	ASP
1	B	339	PHE
1	B	376	MET
1	B	398	ILE
1	B	478	TRP
1	C	9	TYR
1	C	138	ILE
1	C	154	LEU
1	C	182	ASN
1	C	183	TYR
1	C	184	PHE
1	C	212	LEU
1	C	301	PRO
1	C	303	VAL
1	C	316	LEU
1	C	325	ASN
1	C	376	MET
1	C	398	ILE
1	C	478	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 1 ligands modelled in this entry, 1 is 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, 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	442/485 (91%)	1.13	95 (21%) 0 1	32, 111, 172, 239	0
1	B	439/485 (90%)	1.03	88 (20%) 1 1	29, 112, 170, 237	0
1	C	436/485 (89%)	1.08	107 (24%) 0 1	33, 113, 170, 243	0
All	All	1317/1455 (90%)	1.08	290 (22%) 0 1	29, 112, 171, 243	0

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	GLU	11.4
1	A	53	ALA	9.3
1	A	52	ALA	9.3
1	A	54	ASN	9.1
1	C	471	LEU	8.8
1	B	401	ASN	8.5
1	A	471	LEU	8.4
1	B	471	LEU	8.1
1	A	433	SER	7.9
1	A	49	SER	7.8
1	A	85	ARG	7.6
1	A	222	GLU	7.6
1	A	84	ARG	7.2
1	A	432	ASN	7.1
1	A	223	SER	7.0
1	C	399	PHE	6.9
1	B	404	ARG	6.8
1	B	187	ARG	6.7
1	C	401	ASN	6.6
1	C	60	CYS	6.4
1	A	51	SER	6.4
1	A	55	SER	6.2
1	A	274	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	112	ILE	6.1
1	A	475	GLU	6.1
1	C	472	GLU	6.0
1	B	109	PHE	5.9
1	A	221	PRO	5.7
1	A	472	GLU	5.7
1	B	400	PRO	5.7
1	C	400	PRO	5.7
1	C	475	GLU	5.6
1	C	52	ALA	5.6
1	C	63	SER	5.5
1	B	402	ALA	5.5
1	C	64	ALA	5.3
1	A	364	TYR	5.3
1	A	48	LEU	5.3
1	B	110	THR	5.2
1	C	51	SER	5.2
1	C	56	LEU	5.1
1	B	186	ALA	5.0
1	B	403	ILE	4.9
1	A	220	VAL	4.9
1	B	441	ASN	4.9
1	C	55	SER	4.9
1	A	441	ASN	4.9
1	B	45	PRO	4.8
1	C	133	ARG	4.8
1	B	233	GLN	4.8
1	C	48	LEU	4.7
1	B	108	GLY	4.6
1	B	371	VAL	4.6
1	B	370	ILE	4.6
1	C	111	SER	4.6
1	C	119	PRO	4.5
1	C	23	LEU	4.5
1	B	185	ILE	4.5
1	B	472	GLU	4.5
1	A	23	LEU	4.5
1	C	95	PHE	4.4
1	C	403	ILE	4.3
1	B	224	PRO	4.3
1	A	273	PHE	4.3
1	C	380	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	113	ASN	4.3
1	A	154	LEU	4.3
1	B	107	LEU	4.2
1	B	369	GLY	4.2
1	A	272	MET	4.2
1	A	197	ASP	4.2
1	B	442	GLY	4.1
1	A	47	ASN	4.1
1	C	65	LEU	4.1
1	A	150	TYR	4.1
1	B	44	ALA	4.1
1	A	276	GLY	4.1
1	C	376	MET	4.1
1	A	119	PRO	4.1
1	B	221	PRO	4.0
1	C	43	VAL	4.0
1	C	359	LEU	4.0
1	C	59	PHE	4.0
1	C	356	MET	4.0
1	C	42	PHE	4.0
1	A	87	SER	4.0
1	C	398	ILE	3.9
1	A	277	VAL	3.9
1	A	118	VAL	3.9
1	B	57	LEU	3.9
1	A	478	TRP	3.9
1	A	380	VAL	3.9
1	B	379	TYR	3.8
1	C	224	PRO	3.8
1	B	150	TYR	3.8
1	C	46	GLN	3.8
1	C	402	ALA	3.7
1	C	57	LEU	3.7
1	B	380	VAL	3.7
1	C	62	ALA	3.7
1	C	106	GLU	3.7
1	B	359	LEU	3.7
1	C	424	TRP	3.7
1	B	263	GLY	3.6
1	C	363	PHE	3.6
1	B	356	MET	3.6
1	C	53	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	469	LYS	3.6
1	B	54	ASN	3.6
1	A	341	ARG	3.6
1	A	291	VAL	3.6
1	C	129	PHE	3.6
1	B	432	ASN	3.5
1	C	110	THR	3.5
1	B	225	ARG	3.5
1	B	358	SER	3.5
1	A	140	VAL	3.5
1	C	277	VAL	3.5
1	C	254	GLN	3.4
1	B	106	GLU	3.4
1	C	322	GLY	3.4
1	A	275	VAL	3.4
1	B	220	VAL	3.4
1	C	225	ARG	3.4
1	C	139	GLY	3.4
1	A	278	ILE	3.4
1	C	372	ALA	3.4
1	A	56	LEU	3.3
1	A	213	PHE	3.3
1	C	27	ASP	3.3
1	B	430	ASP	3.3
1	B	43	VAL	3.3
1	C	140	VAL	3.3
1	B	335	THR	3.3
1	B	352	MET	3.3
1	B	339	PHE	3.3
1	A	139	GLY	3.3
1	C	474	LEU	3.2
1	B	345	GLN	3.2
1	B	50	GLU	3.2
1	A	199	TRP	3.2
1	A	363	PHE	3.2
1	A	293	ILE	3.2
1	C	442	GLY	3.2
1	C	107	LEU	3.2
1	A	224	PRO	3.2
1	C	255	GLU	3.2
1	B	398	ILE	3.2
1	C	49	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	50	GLU	3.1
1	C	379	TYR	3.1
1	A	43	VAL	3.1
1	C	445	TYR	3.1
1	C	425	THR	3.1
1	C	371	VAL	3.1
1	B	154	LEU	3.0
1	B	448	TYR	3.0
1	B	341	ARG	3.0
1	B	444	SER	3.0
1	B	361	THR	3.0
1	B	291	VAL	3.0
1	A	95	PHE	3.0
1	B	382	ALA	3.0
1	C	136	GLY	3.0
1	B	53	ALA	3.0
1	C	470	THR	3.0
1	B	223	SER	3.0
1	C	428	MET	3.0
1	B	56	LEU	3.0
1	A	138	ILE	3.0
1	B	399	PHE	3.0
1	C	478	TRP	3.0
1	C	146	LEU	3.0
1	C	126	VAL	2.9
1	A	235	GLN	2.9
1	C	154	LEU	2.9
1	A	112	ILE	2.9
1	B	385	MET	2.9
1	A	74	LEU	2.9
1	C	443	PHE	2.9
1	A	399	PHE	2.9
1	A	75	GLY	2.9
1	C	352	MET	2.9
1	C	370	ILE	2.8
1	B	460	TRP	2.8
1	A	466	THR	2.8
1	C	233	GLN	2.8
1	A	398	ILE	2.8
1	A	474	LEU	2.8
1	B	189	GLY	2.8
1	A	196	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	387	TRP	2.8
1	C	105	PRO	2.8
1	C	150	TYR	2.8
1	C	253	VAL	2.8
1	C	122	LEU	2.8
1	C	364	TYR	2.8
1	B	42	PHE	2.7
1	A	345	GLN	2.7
1	B	376	MET	2.7
1	A	91	ALA	2.7
1	B	254	GLN	2.7
1	A	379	TYR	2.7
1	C	407	ALA	2.7
1	A	194	LEU	2.7
1	A	198	GLY	2.6
1	A	200	ARG	2.6
1	B	445	TYR	2.6
1	C	223	SER	2.6
1	C	102	SER	2.6
1	C	476	ALA	2.6
1	A	394	LEU	2.6
1	B	217	LEU	2.6
1	C	404	ARG	2.6
1	B	446	TRP	2.6
1	B	112	ILE	2.6
1	A	86	ASP	2.6
1	A	397	GLU	2.5
1	B	363	PHE	2.5
1	C	280	ILE	2.5
1	B	213	PHE	2.5
1	A	463	VAL	2.5
1	B	201	TYR	2.5
1	A	225	ARG	2.5
1	C	20	GLY	2.5
1	B	88	LEU	2.5
1	A	403	ILE	2.5
1	A	88	LEU	2.5
1	A	217	LEU	2.5
1	C	88	LEU	2.5
1	B	234	GLU	2.4
1	C	430	ASP	2.4
1	B	387	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	193	TRP	2.4
1	C	176	LEU	2.4
1	A	292	GLY	2.4
1	A	226	TRP	2.4
1	B	340	GLY	2.4
1	B	405	GLY	2.4
1	B	475	GLU	2.4
1	C	142	LEU	2.3
1	C	237	GLU	2.3
1	B	52	ALA	2.3
1	B	84	ARG	2.3
1	A	400	PRO	2.3
1	B	188	SER	2.3
1	C	61	VAL	2.3
1	B	362	ALA	2.3
1	A	142	LEU	2.3
1	A	296	VAL	2.3
1	B	46	GLN	2.3
1	C	47	ASN	2.3
1	C	54	ASN	2.3
1	C	209	PRO	2.3
1	C	319	ILE	2.3
1	A	431	LYS	2.3
1	A	70	ILE	2.2
1	C	383	PHE	2.2
1	A	20	GLY	2.2
1	A	465	GLU	2.2
1	A	126	VAL	2.2
1	C	41	VAL	2.2
1	B	443	PHE	2.2
1	C	291	VAL	2.2
1	A	430	ASP	2.2
1	C	382	ALA	2.2
1	C	325	ASN	2.2
1	A	79	SER	2.2
1	C	360	GLY	2.2
1	C	281	GLY	2.1
1	B	193	TRP	2.1
1	A	352	MET	2.1
1	B	317	GLN	2.1
1	C	91	ALA	2.1
1	B	16	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	372	ALA	2.1
1	C	448	TYR	2.1
1	A	464	PRO	2.1
1	C	31	ILE	2.1
1	A	280	ILE	2.1
1	B	338	LYS	2.1
1	A	24	PHE	2.1
1	B	113	ASN	2.1
1	C	38	LEU	2.0
1	C	365	THR	2.0
1	C	441	ASN	2.0
1	B	237	GLU	2.0
1	A	428	MET	2.0
1	A	459	MET	2.0
1	C	317	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 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, 95th 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(\AA^2)	Q<0.9
2	CD	A	501	1/1	0.92	0.23	297,297,297,297	0

6.5 Other polymers [i](#)

There are no such residues in this entry.