



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:43 PM GMT

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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

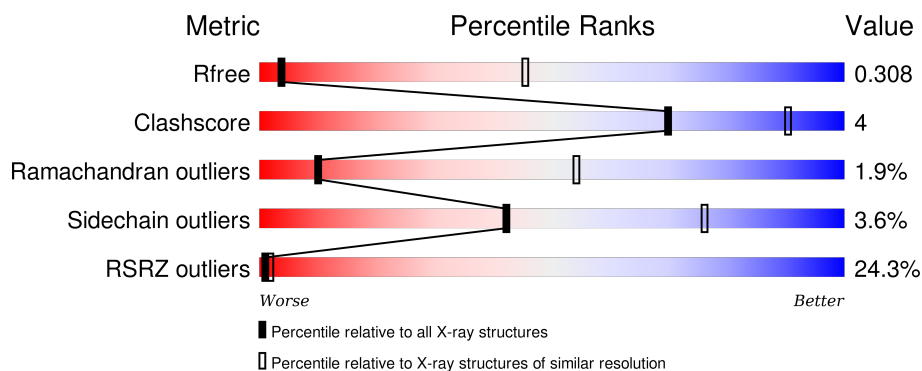
1 Overall quality at a glance

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}	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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 ≥ 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	485	
1	B	485	
1	C	485	

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

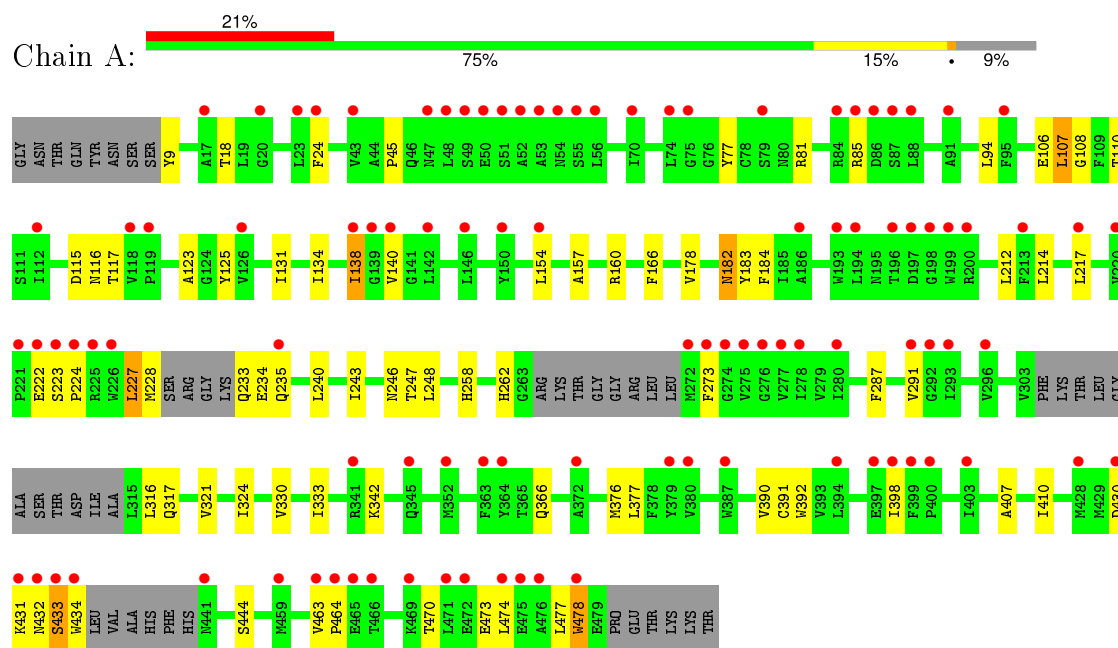
- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

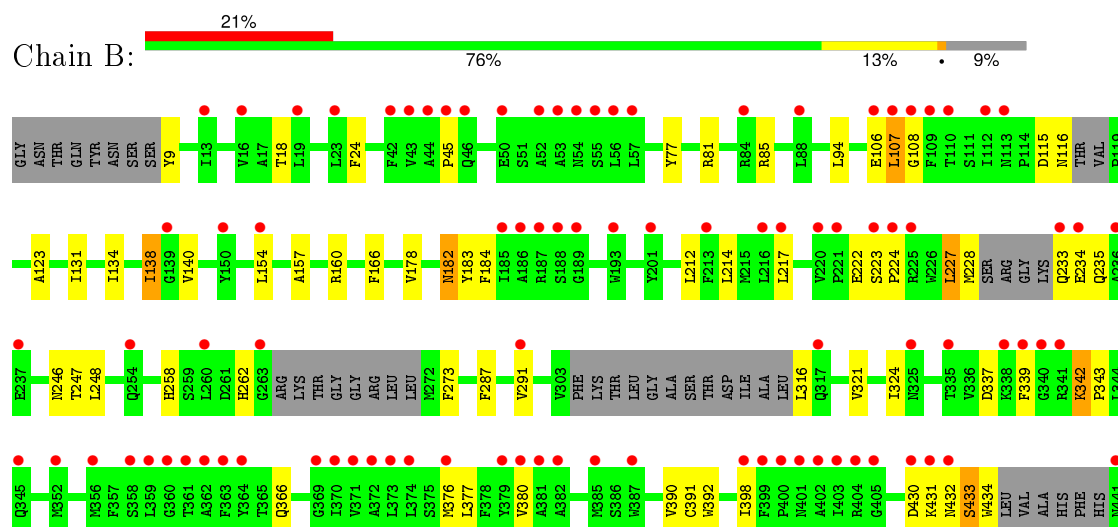
3 Residue-property plots [i](#)

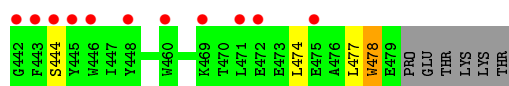
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

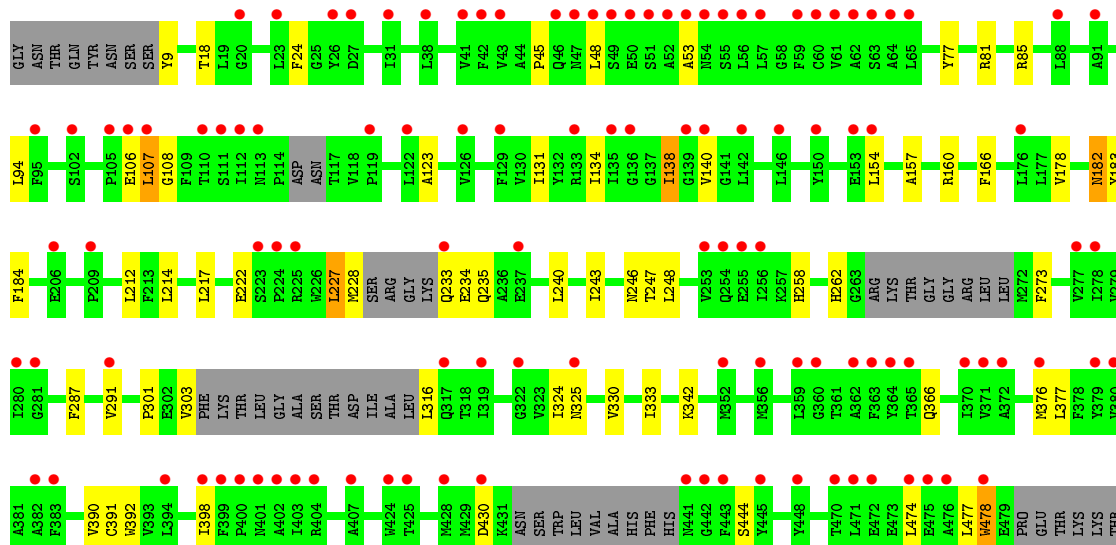
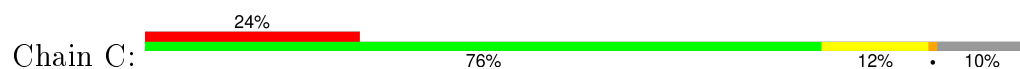


• Molecule 1: D-xylose-proton symporter





● 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 0.287 , 0.308	Depositor DCC
R_{free} test set	1368 reflections (7.65%)	DCC
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 , 140.7	EDS
Estimated twinning fraction	0.085 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 17942 reflections	Xtriage
F_o, F_c correlation	0.62	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, 0.375 respectively for untwinned datasets, and 0.333, 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:C:214:LEU:HA	1:C:217:LEU:HD12	1.94	0.48
1:B:157:ALA:HA	1:B:160:ARG:HE	1.79	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:77:TYR:CZ	1:C:81:ARG:HD2	2.54	0.42
1:C:246:ASN:O	1:C:248:LEU:N	2.52	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:B:106:GLU:HG2	1:B:107:LEU:N	2.34	0.42
1:A:246:ASN:O	1:A:248:LEU:N	2.53	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:C:106:GLU:HG2	1:C:107:LEU:N	2.35	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:48:LEU:H	1:C:53:ALA:HB2	1.85	0.41
1:A:463:VAL:HA	1:A:464:PRO:HD3	1.93	0.41
1:B:342:LYS:HB3	1:B:343:PRO:HD3	2.02	0.41
1:A:77:TYR:CZ	1:A:81:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PRO:HG2	1:A:123:ALA:HB2	2.03	0.41
1:A:258:HIS:CE1	1:B:258:HIS:CD2	3.09	0.41
1:A:407:ALA:HA	1:A:410:ILE:HD12	2.02	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%)	9	52
1	B	427/485 (88%)	393 (92%)	26 (6%)	8 (2%)	10	54
1	C	424/485 (87%)	394 (93%)	23 (5%)	7 (2%)	11	56
All	All	1283/1455 (88%)	1186 (92%)	73 (6%)	24 (2%)	10	54

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%)	47	78
1	B	352/390 (90%)	339 (96%)	13 (4%)	41	75
1	C	349/390 (90%)	335 (96%)	14 (4%)	38	73
All	All	1056/1170 (90%)	1018 (96%)	38 (4%)	42	76

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [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	442/485 (91%)	1.25	101 (22%) 1 2	32, 111, 172, 239	0
1	B	439/485 (90%)	1.15	104 (23%) 1 2	29, 112, 170, 237	0
1	C	436/485 (89%)	1.20	115 (26%) 1 2	33, 113, 170, 243	0
All	All	1317/1455 (90%)	1.20	320 (24%) 1 2	29, 112, 171, 243	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	GLU	11.9
1	A	53	ALA	10.3
1	A	52	ALA	10.2
1	A	54	ASN	9.6
1	C	471	LEU	9.4
1	A	471	LEU	8.9
1	B	471	LEU	8.7
1	B	401	ASN	8.7
1	A	433	SER	8.4
1	A	49	SER	8.2
1	A	222	GLU	7.9
1	A	85	ARG	7.8
1	A	432	ASN	7.4
1	A	84	ARG	7.4
1	C	399	PHE	7.3
1	A	223	SER	7.3
1	B	187	ARG	7.1
1	B	404	ARG	7.0
1	C	401	ASN	6.8
1	A	51	SER	6.8
1	A	55	SER	6.6
1	C	60	CYS	6.6
1	C	112	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	274	GLY	6.5
1	A	475	GLU	6.4
1	B	109	PHE	6.4
1	C	472	GLU	6.3
1	C	52	ALA	6.2
1	A	221	PRO	6.0
1	B	402	ALA	6.0
1	A	472	GLU	6.0
1	C	475	GLU	5.9
1	C	64	ALA	5.8
1	C	63	SER	5.8
1	B	400	PRO	5.8
1	B	186	ALA	5.8
1	B	110	THR	5.8
1	C	400	PRO	5.8
1	A	48	LEU	5.7
1	A	364	TYR	5.7
1	C	56	LEU	5.6
1	C	51	SER	5.6
1	A	220	VAL	5.3
1	C	55	SER	5.3
1	B	403	ILE	5.2
1	B	441	ASN	5.2
1	B	45	PRO	5.1
1	C	48	LEU	5.0
1	B	108	GLY	5.0
1	C	133	ARG	5.0
1	B	185	ILE	5.0
1	A	441	ASN	4.9
1	B	233	GLN	4.9
1	B	370	ILE	4.9
1	C	23	LEU	4.9
1	B	371	VAL	4.9
1	A	23	LEU	4.8
1	C	111	SER	4.8
1	C	95	PHE	4.8
1	B	472	GLU	4.7
1	B	44	ALA	4.6
1	C	119	PRO	4.6
1	C	403	ILE	4.6
1	C	380	VAL	4.6
1	A	154	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	107	LEU	4.6
1	A	273	PHE	4.5
1	A	150	TYR	4.5
1	B	442	GLY	4.5
1	A	197	ASP	4.5
1	C	65	LEU	4.4
1	B	369	GLY	4.4
1	A	47	ASN	4.4
1	A	276	GLY	4.4
1	B	224	PRO	4.4
1	A	272	MET	4.3
1	C	359	LEU	4.3
1	C	376	MET	4.3
1	A	478	TRP	4.3
1	C	59	PHE	4.3
1	C	113	ASN	4.3
1	B	379	TYR	4.3
1	C	356	MET	4.3
1	C	43	VAL	4.2
1	C	42	PHE	4.2
1	C	398	ILE	4.2
1	B	57	LEU	4.2
1	A	277	VAL	4.2
1	B	150	TYR	4.2
1	B	221	PRO	4.2
1	A	380	VAL	4.1
1	A	119	PRO	4.1
1	C	424	TRP	4.1
1	A	118	VAL	4.1
1	A	87	SER	4.1
1	C	53	ALA	4.1
1	C	57	LEU	4.1
1	C	62	ALA	4.1
1	C	402	ALA	4.1
1	B	359	LEU	4.0
1	C	46	GLN	3.9
1	B	356	MET	3.9
1	B	380	VAL	3.9
1	B	263	GLY	3.9
1	C	106	GLU	3.9
1	C	363	PHE	3.9
1	C	224	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	110	THR	3.8
1	C	129	PHE	3.8
1	A	291	VAL	3.8
1	C	372	ALA	3.7
1	A	140	VAL	3.7
1	B	54	ASN	3.7
1	C	277	VAL	3.7
1	B	432	ASN	3.7
1	C	322	GLY	3.7
1	B	106	GLU	3.7
1	A	275	VAL	3.7
1	B	358	SER	3.7
1	B	220	VAL	3.7
1	C	139	GLY	3.7
1	A	278	ILE	3.7
1	B	225	ARG	3.6
1	A	469	LYS	3.6
1	C	254	GLN	3.6
1	A	56	LEU	3.6
1	A	341	ARG	3.6
1	A	199	TRP	3.6
1	B	43	VAL	3.6
1	C	27	ASP	3.6
1	C	140	VAL	3.6
1	B	352	MET	3.6
1	B	430	ASP	3.5
1	C	225	ARG	3.5
1	A	139	GLY	3.5
1	B	335	THR	3.5
1	A	213	PHE	3.5
1	C	379	TYR	3.5
1	B	339	PHE	3.5
1	C	107	LEU	3.5
1	C	425	THR	3.5
1	C	474	LEU	3.5
1	C	445	TYR	3.5
1	C	442	GLY	3.4
1	B	345	GLN	3.4
1	B	448	TYR	3.4
1	B	398	ILE	3.4
1	A	293	ILE	3.4
1	A	363	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	255	GLU	3.4
1	B	382	ALA	3.4
1	C	49	SER	3.3
1	C	50	GLU	3.3
1	A	43	VAL	3.3
1	C	428	MET	3.3
1	B	50	GLU	3.3
1	C	371	VAL	3.3
1	B	53	ALA	3.3
1	C	478	TRP	3.3
1	B	291	VAL	3.3
1	C	136	GLY	3.3
1	A	138	ILE	3.3
1	B	154	LEU	3.3
1	B	361	THR	3.3
1	B	444	SER	3.3
1	A	95	PHE	3.3
1	A	224	PRO	3.2
1	C	146	LEU	3.2
1	A	74	LEU	3.2
1	B	56	LEU	3.2
1	B	341	ARG	3.2
1	C	470	THR	3.2
1	A	112	ILE	3.2
1	C	443	PHE	3.1
1	C	126	VAL	3.1
1	C	154	LEU	3.1
1	C	364	TYR	3.1
1	A	75	GLY	3.1
1	A	196	THR	3.1
1	C	370	ILE	3.1
1	B	189	GLY	3.1
1	B	385	MET	3.1
1	A	235	GLN	3.1
1	B	399	PHE	3.1
1	C	352	MET	3.1
1	A	399	PHE	3.1
1	C	150	TYR	3.1
1	B	223	SER	3.1
1	B	460	TRP	3.1
1	A	474	LEU	3.1
1	B	42	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	398	ILE	3.0
1	A	91	ALA	3.0
1	A	387	TRP	3.0
1	B	445	TYR	3.0
1	C	122	LEU	3.0
1	A	379	TYR	3.0
1	A	466	THR	3.0
1	C	253	VAL	3.0
1	C	476	ALA	3.0
1	C	233	GLN	3.0
1	C	407	ALA	2.9
1	A	194	LEU	2.9
1	A	198	GLY	2.9
1	C	105	PRO	2.9
1	B	376	MET	2.9
1	B	446	TRP	2.9
1	A	200	ARG	2.8
1	A	345	GLN	2.8
1	B	254	GLN	2.8
1	C	102	SER	2.8
1	B	201	TYR	2.8
1	A	394	LEU	2.8
1	B	217	LEU	2.8
1	C	280	ILE	2.8
1	B	363	PHE	2.8
1	B	112	ILE	2.7
1	C	223	SER	2.7
1	B	213	PHE	2.7
1	A	463	VAL	2.7
1	B	88	LEU	2.7
1	C	88	LEU	2.7
1	A	217	LEU	2.7
1	A	88	LEU	2.7
1	C	20	GLY	2.7
1	A	193	TRP	2.7
1	A	403	ILE	2.7
1	A	86	ASP	2.6
1	B	387	TRP	2.6
1	C	176	LEU	2.6
1	A	397	GLU	2.6
1	B	362	ALA	2.6
1	C	142	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	430	ASP	2.6
1	B	52	ALA	2.6
1	C	404	ARG	2.6
1	B	340	GLY	2.6
1	A	226	TRP	2.6
1	A	142	LEU	2.5
1	A	225	ARG	2.5
1	C	54	ASN	2.5
1	B	188	SER	2.5
1	B	234	GLU	2.5
1	C	319	ILE	2.5
1	B	84	ARG	2.5
1	C	237	GLU	2.5
1	A	292	GLY	2.5
1	B	405	GLY	2.5
1	C	382	ALA	2.5
1	B	46	GLN	2.5
1	A	70	ILE	2.5
1	C	61	VAL	2.5
1	B	193	TRP	2.4
1	B	475	GLU	2.4
1	C	91	ALA	2.4
1	C	383	PHE	2.4
1	A	296	VAL	2.4
1	C	448	TYR	2.4
1	B	443	PHE	2.4
1	A	400	PRO	2.4
1	A	126	VAL	2.4
1	C	291	VAL	2.4
1	A	20	GLY	2.4
1	C	47	ASN	2.4
1	C	209	PRO	2.4
1	C	281	GLY	2.3
1	B	372	ALA	2.3
1	C	360	GLY	2.3
1	A	430	ASP	2.3
1	C	41	VAL	2.3
1	A	465	GLU	2.3
1	A	280	ILE	2.3
1	A	352	MET	2.3
1	B	16	VAL	2.3
1	C	325	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	SER	2.3
1	A	431	LYS	2.3
1	B	317	GLN	2.3
1	A	428	MET	2.3
1	C	365	THR	2.3
1	A	24	PHE	2.2
1	C	31	ILE	2.2
1	C	26	TYR	2.2
1	C	38	LEU	2.2
1	B	13	ILE	2.2
1	B	216	LEU	2.2
1	A	459	MET	2.2
1	A	476	ALA	2.2
1	A	17	ALA	2.2
1	C	206	GLU	2.2
1	A	464	PRO	2.2
1	A	146	LEU	2.2
1	B	381	ALA	2.2
1	B	373	LEU	2.2
1	C	256	ILE	2.1
1	C	441	ASN	2.1
1	A	186	ALA	2.1
1	C	317	GLN	2.1
1	B	236	ALA	2.1
1	B	364	TYR	2.1
1	B	237	GLU	2.1
1	C	153	GLU	2.1
1	B	113	ASN	2.1
1	B	19	LEU	2.1
1	B	338	LYS	2.1
1	B	360	GLY	2.1
1	B	431	LYS	2.1
1	C	135	ILE	2.1
1	B	139	GLY	2.1
1	C	362	ALA	2.1
1	C	394	LEU	2.1
1	A	434	TRP	2.1
1	B	325	ASN	2.1
1	B	374	LEU	2.1
1	B	55	SER	2.0
1	A	372	ALA	2.0
1	C	278	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	23	LEU	2.0
1	B	260	LEU	2.0
1	B	469	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CD	A	501	1/1	0.92	0.23	-0.62	297,297,297,297	0

6.5 Other polymers [i](#)

There are no such residues in this entry.