



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:05 AM UTC

PDB ID : 4JA4 / pdb_00004ja4
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 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

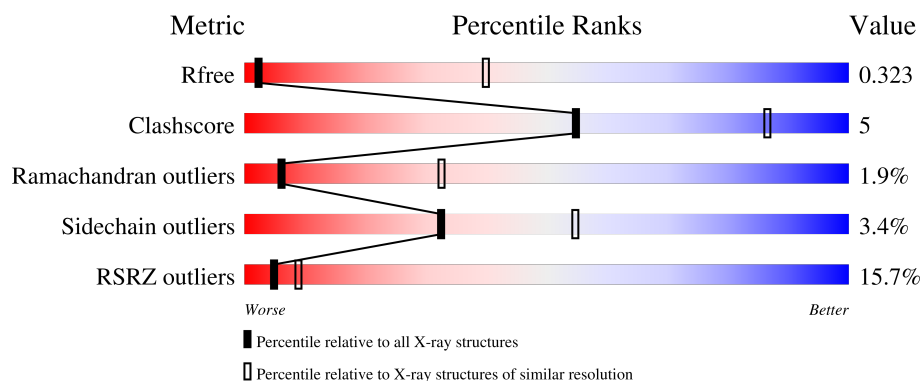
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	485	14% 75% 15% • 9%
1	B	485	15% 76% 13% • 9%
1	C	485	14% 76% 12% • 10%

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

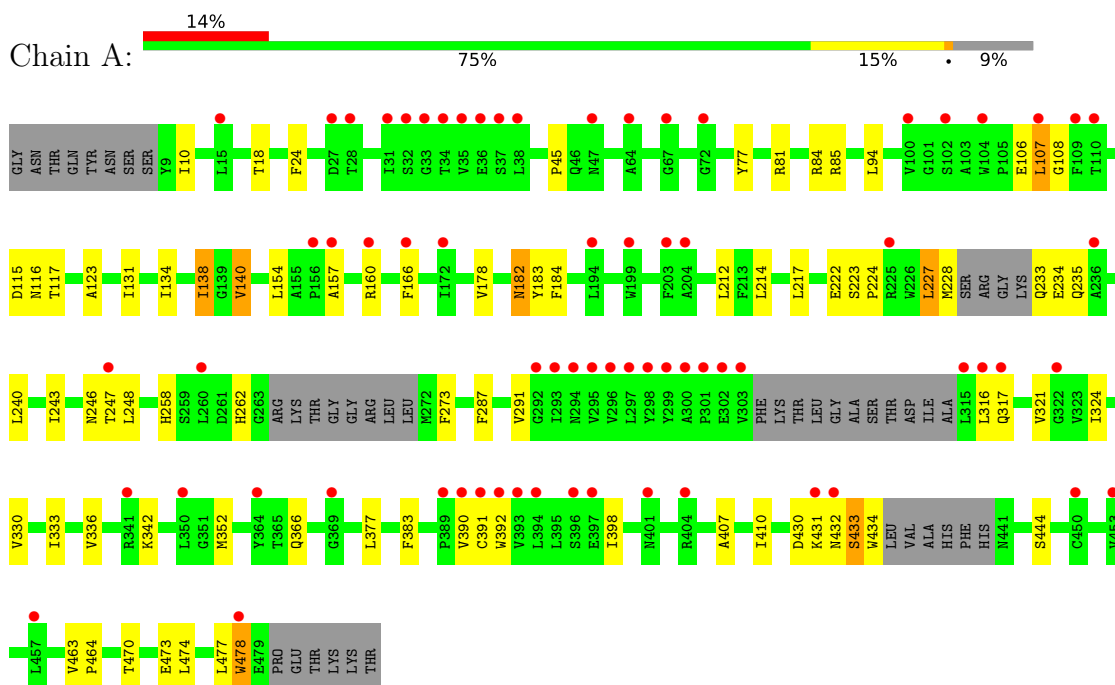
- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

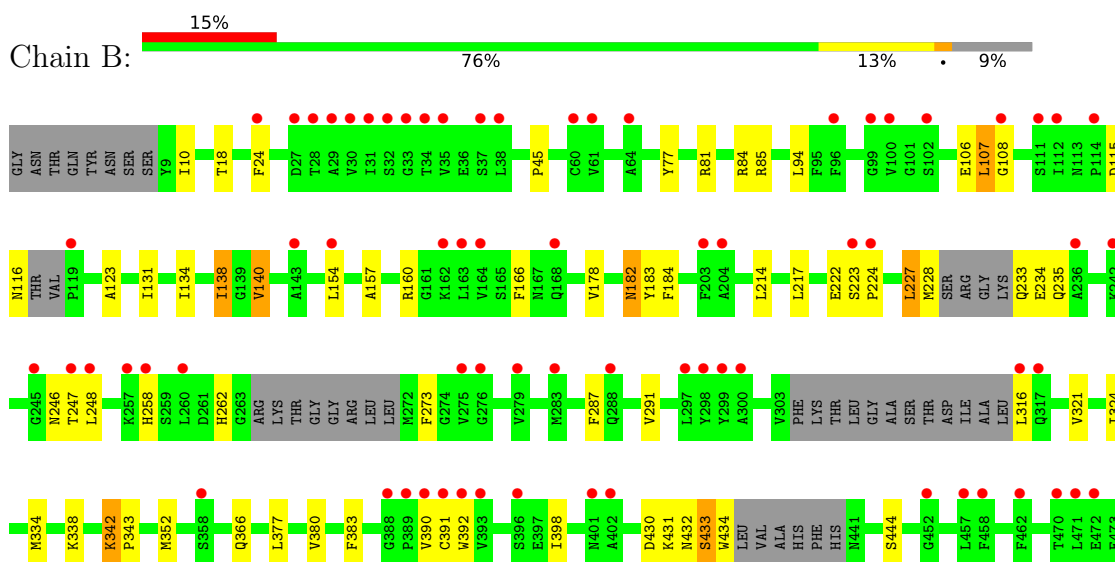
3 Residue-property plots [i](#)

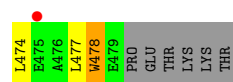
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

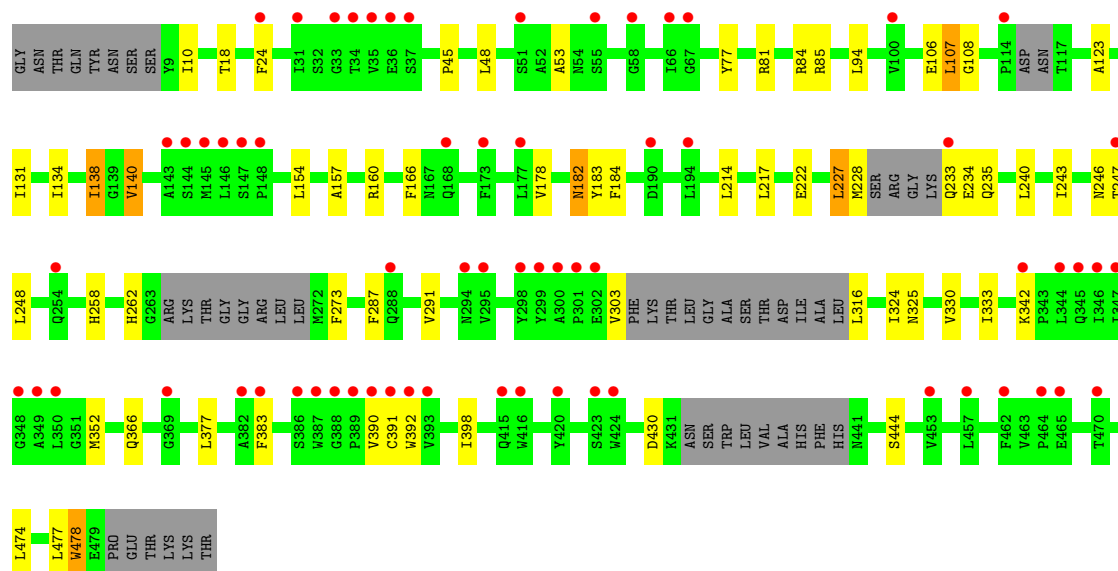
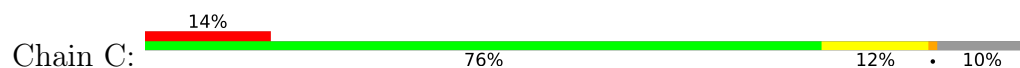


• Molecule 1: D-xylose-proton symporter





● 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 41.18 – 4.20	Depositor EDS
% Data completeness (in resolution range)	72.2 (41.18-4.20) 72.3 (41.18-4.20)	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 0.299 , 0.323	Depositor DCC
R_{free} test set	1374 reflections (5.54%)	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)	0.25 , 109.1	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	0.82	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	0.30	0/3488	0.73	1/4745 (0.0%)
1	B	0.30	0/3465	0.72	0/4710
1	C	0.30	0/3433	0.72	0/4667
All	All	0.30	0/10386	0.73	1/14122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	VAL	N-CA-C	5.38	115.52	110.30

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	37	0
1	B	3379	0	3418	33	0
1	C	3349	0	3402	28	0
2	A	1	0	0	0	0
All	All	10130	0	10265	97	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 5.

All (97) 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:291:VAL:HG11	1:C:352:MET:HE2	1.81	0.61
1:C:178:VAL:O	1:C:182:ASN:ND2	2.33	0.60
1:A:291:VAL:HG11	1:A:352:MET:HE2	1.83	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:B:291:VAL:HG11	1:B:352:MET:HE2	1.84	0.58
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:B:352:MET:HE1	1:B:383:PHE:HD2	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:352:MET:HE1	1:C:383:PHE:HD2	1.70	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:A:352:MET:HE1	1:A:383:PHE:HD2	1.71	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:334:MET:HE3	1:B:338:LYS:HE3	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:24:PHE:CD1	1:A:140:VAL:HG13	2.55	0.41
1:A:106:GLU:HG2	1:A:107:LEU:N	2.35	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
1:A:77:TYR:CZ	1:A:81:ARG:HD2	2.56	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

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	432/485 (89%)	399 (92%)	24 (6%)	9 (2%)	5	30
1	B	427/485 (88%)	393 (92%)	26 (6%)	8 (2%)	6	32
1	C	424/485 (87%)	394 (93%)	23 (5%)	7 (2%)	7	35
All	All	1283/1455 (88%)	1186 (92%)	73 (6%)	24 (2%)	6	32

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
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%)	343 (97%)	12 (3%)	32	55
1	B	352/390 (90%)	341 (97%)	11 (3%)	35	56
1	C	349/390 (90%)	336 (96%)	13 (4%)	30	51
All	All	1056/1170 (90%)	1020 (97%)	36 (3%)	32	55

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	84	ARG
1	A	138	ILE
1	A	140	VAL
1	A	154	LEU
1	A	182	ASN
1	A	183	TYR
1	A	184	PHE
1	A	212	LEU
1	A	316	LEU
1	A	398	ILE
1	A	478	TRP
1	B	10	ILE
1	B	84	ARG
1	B	138	ILE
1	B	140	VAL
1	B	154	LEU
1	B	182	ASN
1	B	183	TYR
1	B	184	PHE
1	B	316	LEU
1	B	398	ILE
1	B	478	TRP
1	C	10	ILE
1	C	84	ARG
1	C	138	ILE
1	C	140	VAL
1	C	154	LEU
1	C	182	ASN
1	C	183	TYR
1	C	184	PHE
1	C	303	VAL
1	C	316	LEU
1	C	325	ASN
1	C	398	ILE
1	C	478	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	251	GLN
1	A	294	ASN

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Mol	Chain	Res	Type
1	A	415	GLN
1	A	432	ASN
1	B	39	ASN
1	B	432	ASN
1	C	39	ASN
1	C	441	ASN

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 oligosaccharides 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%)	0.85	70 (15%) 5 9	32, 111, 172, 239	0
1	B	439/485 (90%)	0.87	71 (16%) 4 8	29, 112, 170, 237	0
1	C	436/485 (89%)	0.76	66 (15%) 5 9	33, 113, 170, 243	0
All	All	1317/1455 (90%)	0.83	207 (15%) 5 9	29, 112, 171, 243	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	392	TRP	17.2
1	A	302	GLU	16.1
1	A	299	TYR	15.1
1	A	301	PRO	13.8
1	B	30	VAL	13.0
1	C	392	TRP	12.6
1	B	389	PRO	12.1
1	C	389	PRO	11.3
1	A	296	VAL	9.8
1	B	31	ILE	9.6
1	B	32	SER	9.6
1	A	298	TYR	9.3
1	A	295	VAL	9.3
1	B	462	PHE	9.0
1	B	33	GLY	8.6
1	B	298	TYR	8.5
1	B	34	THR	8.4
1	A	393	VAL	7.8
1	C	350	LEU	7.7
1	A	33	GLY	7.4
1	A	300	ALA	7.1
1	C	391	CYS	6.9
1	C	345	GLN	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	247	THR	6.9
1	C	36	GLU	6.9
1	A	294	ASN	6.8
1	C	144	SER	6.6
1	A	35	VAL	6.5
1	A	34	THR	6.4
1	A	36	GLU	6.3
1	A	392	TRP	6.0
1	B	472	GLU	6.0
1	B	391	CYS	5.9
1	A	390	VAL	5.7
1	C	298	TYR	5.7
1	A	32	SER	5.6
1	C	390	VAL	5.5
1	B	471	LEU	5.5
1	A	293	ILE	5.4
1	C	457	LEU	5.4
1	C	145	MET	5.3
1	C	347	ILE	5.2
1	B	402	ALA	5.1
1	C	388	GLY	5.1
1	A	225	ARG	5.0
1	B	100	VAL	5.0
1	B	288	GLN	5.0
1	C	299	TYR	4.9
1	C	33	GLY	4.8
1	C	302	GLU	4.8
1	B	29	ALA	4.8
1	A	389	PRO	4.7
1	A	431	LYS	4.7
1	C	35	VAL	4.6
1	C	254	GLN	4.6
1	A	297	LEU	4.6
1	C	148	PRO	4.6
1	B	38	LEU	4.5
1	C	31	ILE	4.5
1	A	157	ALA	4.4
1	B	28	THR	4.4
1	B	27	ASP	4.4
1	B	24	PHE	4.4
1	B	168	GLN	4.3
1	B	393	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	450	CYS	4.3
1	A	404	ARG	4.3
1	B	388	GLY	4.3
1	B	299	TYR	4.1
1	C	301	PRO	4.1
1	A	37	SER	4.1
1	C	348	GLY	4.1
1	C	386	SER	4.0
1	B	390	VAL	4.0
1	A	109	PHE	4.0
1	C	464	PRO	4.0
1	A	401	ASN	3.9
1	C	346	ILE	3.9
1	A	394	LEU	3.9
1	C	344	LEU	3.9
1	C	470	THR	3.8
1	B	99	GLY	3.8
1	C	34	THR	3.8
1	B	35	VAL	3.8
1	B	164	VAL	3.8
1	B	470	THR	3.7
1	A	31	ILE	3.7
1	B	203	PHE	3.7
1	B	475	GLU	3.7
1	A	107	LEU	3.7
1	C	146	LEU	3.7
1	A	194	LEU	3.6
1	A	432	ASN	3.6
1	C	383	PHE	3.6
1	A	397	GLU	3.6
1	A	303	VAL	3.6
1	C	168	GLN	3.5
1	A	292	GLY	3.4
1	A	166	PHE	3.4
1	C	24	PHE	3.4
1	C	349	ALA	3.3
1	C	387	TRP	3.3
1	A	317	GLN	3.3
1	C	393	VAL	3.2
1	B	223	SER	3.2
1	B	401	ASN	3.2
1	C	382	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	156	PRO	3.2
1	A	364	TYR	3.1
1	C	300	ALA	3.1
1	C	369	GLY	3.0
1	A	391	CYS	3.0
1	B	102	SER	3.0
1	A	453	VAL	3.0
1	B	260	LEU	3.0
1	B	112	ILE	2.9
1	A	104	TRP	2.9
1	A	27	ASP	2.9
1	A	72	GLY	2.9
1	C	423	SER	2.9
1	C	465	GLU	2.9
1	B	64	ALA	2.9
1	C	66	ILE	2.9
1	A	199	TRP	2.9
1	C	233	GLN	2.9
1	B	143	ALA	2.8
1	A	350	LEU	2.8
1	B	317	GLN	2.8
1	A	341	ARG	2.8
1	A	64	ALA	2.8
1	B	37	SER	2.8
1	B	242	LYS	2.8
1	C	288	GLN	2.8
1	B	96	PHE	2.8
1	C	190	ASP	2.8
1	B	114	PRO	2.8
1	A	322	GLY	2.7
1	B	457	LEU	2.7
1	C	55	SER	2.7
1	B	452	GLY	2.7
1	A	38	LEU	2.7
1	C	194	LEU	2.7
1	B	111	SER	2.7
1	B	247	THR	2.7
1	C	177	LEU	2.7
1	A	204	ALA	2.7
1	B	60	CYS	2.7
1	C	295	VAL	2.7
1	B	257	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	316	LEU	2.7
1	B	396	SER	2.7
1	B	279	VAL	2.6
1	B	119	PRO	2.6
1	B	162	LYS	2.6
1	B	245	GLY	2.6
1	B	316	LEU	2.6
1	A	15	LEU	2.6
1	B	275	VAL	2.6
1	A	47	ASN	2.5
1	A	28	THR	2.5
1	A	110	THR	2.5
1	B	300	ALA	2.5
1	B	154	LEU	2.4
1	A	160	ARG	2.4
1	B	163	LEU	2.4
1	B	248	LEU	2.4
1	B	458	PHE	2.4
1	A	100	VAL	2.4
1	C	424	TRP	2.4
1	A	369	GLY	2.4
1	C	247	THR	2.4
1	B	61	VAL	2.4
1	C	143	ALA	2.4
1	C	114	PRO	2.3
1	C	342	LYS	2.3
1	A	260	LEU	2.3
1	B	283	MET	2.3
1	B	108	GLY	2.3
1	C	453	VAL	2.3
1	C	416	TRP	2.3
1	A	203	PHE	2.3
1	C	58	GLY	2.3
1	C	67	GLY	2.3
1	C	173	PHE	2.3
1	C	415	GLN	2.3
1	C	462	PHE	2.3
1	A	315	LEU	2.2
1	B	204	ALA	2.2
1	B	224	PRO	2.2
1	B	297	LEU	2.2
1	B	258	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	457	LEU	2.2
1	A	478	TRP	2.2
1	A	236	ALA	2.2
1	B	236	ALA	2.2
1	C	100	VAL	2.2
1	A	172	ILE	2.1
1	C	294	ASN	2.1
1	A	67	GLY	2.1
1	B	358	SER	2.1
1	B	276	GLY	2.1
1	C	147	SER	2.1
1	C	420	TYR	2.1
1	A	396	SER	2.1
1	C	37	SER	2.1
1	C	51	SER	2.1
1	A	102	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](#)

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(Å ²)	Q<0.9
2	CD	A	501	1/1	0.93	0.12	297,297,297,297	0

6.5 Other polymers [i](#)

There are no such residues in this entry.