



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:41 PM UTC

PDB ID : 2XUT / pdb_00002xut
Title : Crystal structure of a proton dependent oligopeptide (POT) family transporter.
Authors : Newstead, S.; Drew, D.; Cameron, A.D.; Postis, V.L.; Xia, X.; Fowler, P.W.; Ingram, J.C.; Carpenter, E.P.; Sansom, M.S.P.; McPherson, M.J.; Baldwin, S.A.; Iwata, S.
Deposited on : 2010-10-21
Resolution : 3.62 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

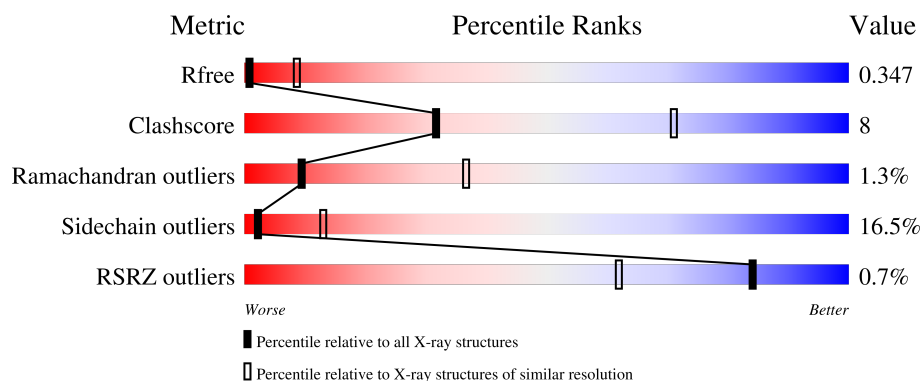
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	524	
1	B	524	
1	C	524	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10533 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 PROTON/PEPTIDE SYMPORTER FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3511	2345	553	589	24			
1	B	456	Total	C	N	O	S	0	0	0
			3511	2345	553	589	24			
1	C	456	Total	C	N	O	S	0	0	0
			3511	2345	553	589	24			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	517	GLY	-	expression tag	UNP Q8EKT7
A	518	SER	-	expression tag	UNP Q8EKT7
A	519	GLU	-	expression tag	UNP Q8EKT7
A	520	ASN	-	expression tag	UNP Q8EKT7
A	521	LEU	-	expression tag	UNP Q8EKT7
A	522	TYR	-	expression tag	UNP Q8EKT7
A	523	PHE	-	expression tag	UNP Q8EKT7
A	524	GLN	-	expression tag	UNP Q8EKT7
A	2	ASN	THR	engineered mutation	UNP Q8EKT7
A	3	SER	THR	engineered mutation	UNP Q8EKT7
B	517	GLY	-	expression tag	UNP Q8EKT7
B	518	SER	-	expression tag	UNP Q8EKT7
B	519	GLU	-	expression tag	UNP Q8EKT7
B	520	ASN	-	expression tag	UNP Q8EKT7
B	521	LEU	-	expression tag	UNP Q8EKT7
B	522	TYR	-	expression tag	UNP Q8EKT7
B	523	PHE	-	expression tag	UNP Q8EKT7
B	524	GLN	-	expression tag	UNP Q8EKT7
B	2	ASN	THR	engineered mutation	UNP Q8EKT7
B	3	SER	THR	engineered mutation	UNP Q8EKT7
C	517	GLY	-	expression tag	UNP Q8EKT7
C	518	SER	-	expression tag	UNP Q8EKT7
C	519	GLU	-	expression tag	UNP Q8EKT7

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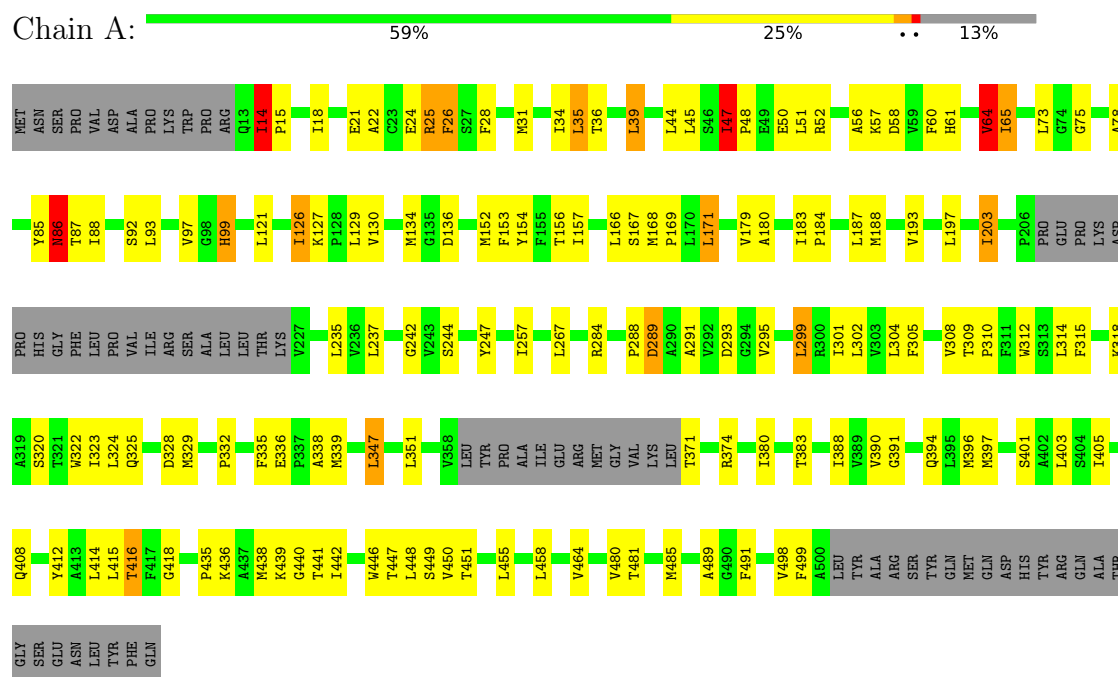
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Chain	Residue	Modelled	Actual	Comment	Reference
C	520	ASN	-	expression tag	UNP Q8EKT7
C	521	LEU	-	expression tag	UNP Q8EKT7
C	522	TYR	-	expression tag	UNP Q8EKT7
C	523	PHE	-	expression tag	UNP Q8EKT7
C	524	GLN	-	expression tag	UNP Q8EKT7
C	2	ASN	THR	engineered mutation	UNP Q8EKT7
C	3	SER	THR	engineered mutation	UNP Q8EKT7

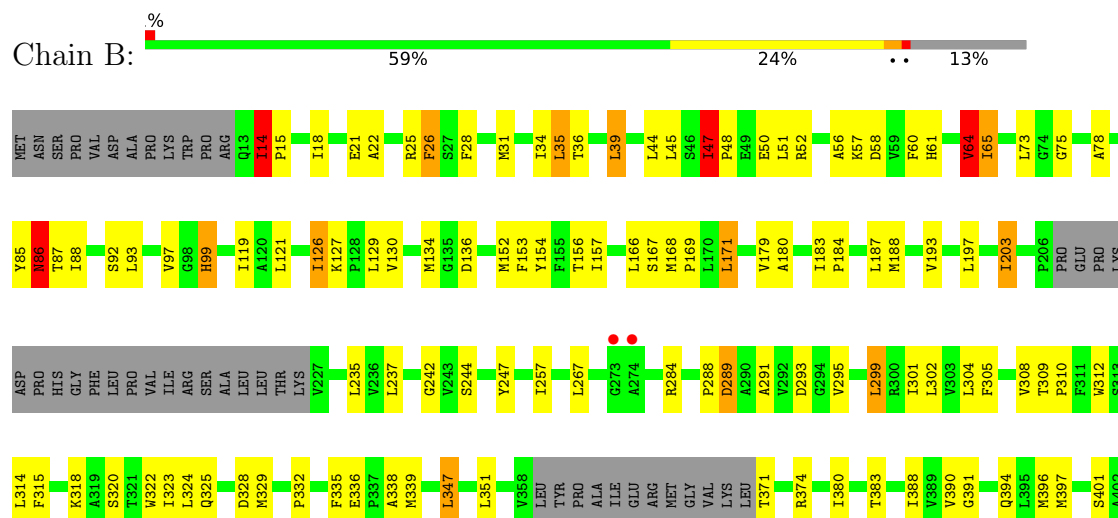
3 Residue-property plots

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.

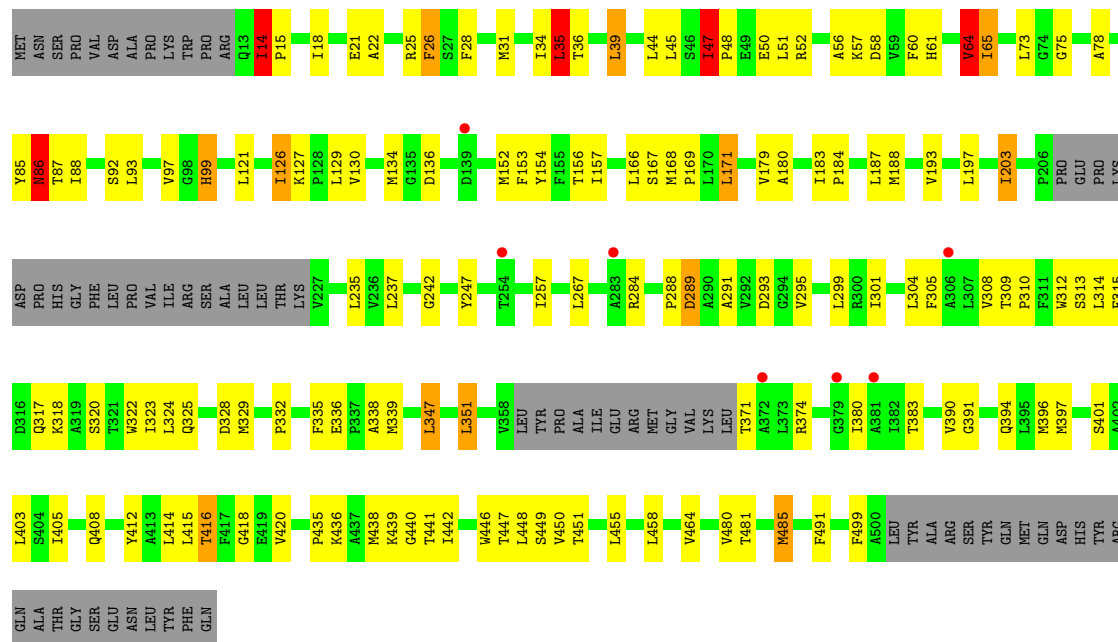
• Molecule 1: PROTON/PEPTIDE SYMPORTER FAMILY PROTEIN



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	159.40Å 159.40Å 152.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.47 – 3.62 35.47 – 3.62	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.47-3.62) 58.5 (35.47-3.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 3.66Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.277 , 0.296 0.323 , 0.347	Depositor DCC
R_{free} test set	1688 reflections (5.84%)	wwPDB-VP
Wilson B-factor (Å ²)	118.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 615.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.110 for -h,-k,l 0.135 for h,-h-k,-l 0.139 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10533	wwPDB-VP
Average B, all atoms (Å ²)	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.74% 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	0.83	2/3604 (0.1%)	1.45	23/4893 (0.5%)
1	B	0.84	2/3604 (0.1%)	1.45	21/4893 (0.4%)
1	C	0.83	1/3604 (0.0%)	1.45	20/4893 (0.4%)
All	All	0.83	5/10812 (0.0%)	1.45	64/14679 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	ILE	CA-C	5.55	1.58	1.52
1	B	14	ILE	CA-C	5.41	1.58	1.52
1	C	14	ILE	CA-C	5.23	1.58	1.52
1	A	99	HIS	CD2-NE2	-5.03	1.32	1.37
1	B	99	HIS	ND1-CE1	5.00	1.37	1.32

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	HIS	CB-CG-CD2	-7.65	121.26	131.20
1	B	99	HIS	CB-CG-CD2	-7.48	121.47	131.20
1	C	99	HIS	CB-CG-CD2	-7.47	121.49	131.20
1	B	86	ASN	CA-CB-CG	6.65	119.25	112.60
1	C	86	ASN	CA-CB-CG	6.63	119.23	112.60
1	A	86	ASN	CA-CB-CG	6.62	119.22	112.60
1	B	35	LEU	N-CA-C	6.44	118.84	111.11
1	C	35	LEU	N-CA-C	6.38	118.77	111.11
1	A	35	LEU	N-CA-C	6.38	118.77	111.11
1	B	408	GLN	N-CA-C	-6.38	107.35	114.62
1	A	408	GLN	N-CA-C	-6.37	107.36	114.62
1	C	408	GLN	N-CA-C	-6.33	107.40	114.62
1	C	449	SER	N-CA-C	-6.18	105.90	113.50
1	B	449	SER	N-CA-C	-6.14	105.94	113.50
1	C	58	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	58	ASP	CA-CB-CG	6.07	118.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	449	SER	N-CA-C	-5.98	106.14	113.50
1	B	57	LYS	CA-C-N	5.81	128.06	120.28
1	B	57	LYS	C-N-CA	5.81	128.06	120.28
1	C	57	LYS	CA-C-N	5.69	127.90	120.28
1	C	57	LYS	C-N-CA	5.69	127.90	120.28
1	B	26	PHE	CA-CB-CG	5.67	119.47	113.80
1	A	26	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	57	LYS	CA-C-N	5.64	127.83	120.28
1	A	57	LYS	C-N-CA	5.64	127.83	120.28
1	A	25	ARG	N-CA-C	5.62	117.40	111.28
1	B	288	PRO	N-CA-C	5.54	119.93	111.11
1	A	288	PRO	N-CA-C	5.52	119.89	111.11
1	C	26	PHE	CA-CB-CG	5.51	119.31	113.80
1	C	64	VAL	N-CA-CB	5.48	120.02	110.65
1	C	288	PRO	N-CA-C	5.45	119.78	111.11
1	C	418	GLY	CA-C-N	5.43	128.01	120.29
1	C	418	GLY	C-N-CA	5.43	128.01	120.29
1	C	65	ILE	CA-C-N	5.43	126.11	120.03
1	C	65	ILE	C-N-CA	5.43	126.11	120.03
1	B	44	LEU	CA-C-N	5.42	128.29	120.38
1	B	44	LEU	C-N-CA	5.42	128.29	120.38
1	B	418	GLY	CA-C-N	5.41	127.98	120.29
1	B	418	GLY	C-N-CA	5.41	127.98	120.29
1	B	64	VAL	N-CA-CB	5.36	119.81	110.65
1	A	65	ILE	CA-C-N	5.36	126.03	120.03
1	A	65	ILE	C-N-CA	5.36	126.03	120.03
1	A	418	GLY	CA-C-N	5.34	127.88	120.29
1	A	418	GLY	C-N-CA	5.34	127.88	120.29
1	B	65	ILE	CA-C-N	5.30	125.96	120.03
1	B	65	ILE	C-N-CA	5.30	125.96	120.03
1	C	44	LEU	CA-C-N	5.15	127.90	120.38
1	C	44	LEU	C-N-CA	5.15	127.90	120.38
1	A	44	LEU	CA-C-N	5.12	127.85	120.38
1	A	44	LEU	C-N-CA	5.12	127.85	120.38
1	B	119	ILE	N-CA-C	-5.11	105.73	110.53
1	A	24	GLU	CB-CG-CD	5.09	121.26	112.60
1	A	242	GLY	CA-C-N	5.09	127.08	120.56
1	A	242	GLY	C-N-CA	5.09	127.08	120.56
1	C	242	GLY	CA-C-N	5.08	127.06	120.56
1	C	242	GLY	C-N-CA	5.08	127.06	120.56
1	C	25	ARG	N-CA-C	5.04	117.51	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	ARG	N-CA-C	5.04	117.50	111.71
1	B	242	GLY	CA-C-N	5.04	127.01	120.56
1	B	242	GLY	C-N-CA	5.04	127.01	120.56
1	A	64	VAL	N-CA-CB	5.03	119.87	110.77
1	A	498	VAL	CA-C-N	5.01	127.25	120.38
1	A	498	VAL	C-N-CA	5.01	127.25	120.38

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	3511	0	3592	58	0
1	B	3511	0	3592	58	0
1	C	3511	0	3592	57	0
All	All	10533	0	10776	173	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 8.

All (173) 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:14:ILE:H	1:B:15:PRO:HD2	1.39	0.87
1:A:14:ILE:H	1:A:15:PRO:HD2	1.40	0.87
1:C:14:ILE:H	1:C:15:PRO:HD2	1.39	0.87
1:A:48:PRO:HD2	1:A:51:LEU:HB2	1.59	0.84
1:B:48:PRO:HD2	1:B:51:LEU:HB2	1.59	0.84
1:C:48:PRO:HD2	1:C:51:LEU:HB2	1.59	0.82
1:A:318:LYS:HA	1:A:322:TRP:CD1	2.26	0.71
1:C:318:LYS:HA	1:C:322:TRP:CD1	2.26	0.70
1:B:318:LYS:HA	1:B:322:TRP:CD1	2.27	0.70
1:C:14:ILE:H	1:C:15:PRO:CD	2.05	0.69
1:A:14:ILE:H	1:A:15:PRO:CD	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ILE:H	1:B:15:PRO:CD	2.05	0.68
1:A:134:MET:HE1	1:A:153:PHE:CD1	2.29	0.68
1:C:134:MET:HE1	1:C:153:PHE:CD1	2.30	0.67
1:C:435:PRO:HB2	1:C:438:MET:HB3	1.76	0.67
1:A:329:MET:HE3	1:A:397:MET:HG2	1.77	0.66
1:B:329:MET:HE3	1:B:397:MET:HG2	1.77	0.66
1:C:329:MET:HE3	1:C:397:MET:HG2	1.77	0.66
1:B:435:PRO:HB2	1:B:438:MET:HB3	1.77	0.66
1:B:134:MET:HE1	1:B:153:PHE:CD1	2.30	0.66
1:A:435:PRO:HB2	1:A:438:MET:HB3	1.77	0.65
1:A:347:LEU:HB3	1:A:416:THR:HG21	1.82	0.61
1:A:56:ALA:O	1:A:60:PHE:HB3	2.00	0.61
1:B:28:PHE:CE2	1:B:127:LYS:NZ	2.64	0.61
1:B:347:LEU:HB3	1:B:416:THR:HG21	1.82	0.61
1:C:347:LEU:HB3	1:C:416:THR:HG21	1.83	0.61
1:B:18:ILE:HG21	1:B:152:MET:HB3	1.82	0.61
1:C:56:ALA:O	1:C:60:PHE:HB3	2.01	0.61
1:B:56:ALA:O	1:B:60:PHE:HB3	2.01	0.61
1:A:18:ILE:HG21	1:A:152:MET:HB3	1.83	0.60
1:C:18:ILE:HG21	1:C:152:MET:HB3	1.82	0.60
1:C:47:ILE:HB	1:C:48:PRO:HD3	1.84	0.59
1:A:47:ILE:HB	1:A:48:PRO:HD3	1.84	0.59
1:A:28:PHE:CE2	1:A:127:LYS:NZ	2.67	0.58
1:C:28:PHE:CE2	1:C:127:LYS:NZ	2.67	0.58
1:B:47:ILE:HB	1:B:48:PRO:HD3	1.85	0.57
1:A:171:LEU:HD23	1:A:180:ALA:HA	1.87	0.56
1:B:171:LEU:HD23	1:B:180:ALA:HA	1.87	0.56
1:C:171:LEU:HD23	1:C:180:ALA:HA	1.88	0.56
1:A:31:MET:HE2	1:A:99:HIS:CE1	2.41	0.56
1:A:136:ASP:HB3	1:A:203:ILE:HD11	1.89	0.55
1:C:47:ILE:HB	1:C:48:PRO:CD	2.38	0.54
1:B:136:ASP:HB3	1:B:203:ILE:HD11	1.89	0.54
1:A:47:ILE:HB	1:A:48:PRO:CD	2.38	0.54
1:C:136:ASP:HB3	1:C:203:ILE:HD11	1.90	0.54
1:B:47:ILE:HB	1:B:48:PRO:CD	2.38	0.54
1:C:184:PRO:HA	1:C:187:LEU:HD12	1.91	0.53
1:B:14:ILE:N	1:B:15:PRO:HD2	2.18	0.53
1:A:184:PRO:HA	1:A:187:LEU:HD12	1.91	0.53
1:B:31:MET:HE2	1:B:99:HIS:CE1	2.43	0.53
1:B:75:GLY:HA2	1:B:78:ALA:HB3	1.91	0.53
1:B:184:PRO:HA	1:B:187:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:MET:HE2	1:C:99:HIS:CE1	2.43	0.53
1:A:126:ILE:O	1:A:129:LEU:HB2	2.09	0.52
1:A:75:GLY:HA2	1:A:78:ALA:HB3	1.91	0.52
1:C:14:ILE:N	1:C:15:PRO:HD2	2.18	0.52
1:C:126:ILE:O	1:C:129:LEU:HB2	2.10	0.52
1:C:34:ILE:HD11	1:C:168:MET:HG3	1.90	0.52
1:C:75:GLY:HA2	1:C:78:ALA:HB3	1.92	0.51
1:A:34:ILE:HD11	1:A:168:MET:HG3	1.91	0.51
1:B:188:MET:HA	1:B:188:MET:HE2	1.93	0.51
1:C:315:PHE:O	1:C:318:LYS:HG2	2.10	0.51
1:B:34:ILE:HD11	1:B:168:MET:HG3	1.91	0.51
1:A:295:VAL:HG11	1:A:438:MET:HE3	1.93	0.50
1:A:315:PHE:O	1:A:318:LYS:HG2	2.11	0.50
1:B:315:PHE:O	1:B:318:LYS:HG2	2.11	0.50
1:B:126:ILE:O	1:B:129:LEU:HB2	2.11	0.50
1:A:14:ILE:N	1:A:15:PRO:HD2	2.19	0.50
1:C:22:ALA:HA	1:C:156:THR:HG23	1.94	0.50
1:C:295:VAL:HG11	1:C:438:MET:HE3	1.93	0.50
1:A:188:MET:HE2	1:A:188:MET:HA	1.93	0.50
1:C:86:ASN:ND2	1:C:86:ASN:H	2.10	0.50
1:A:86:ASN:ND2	1:A:86:ASN:H	2.10	0.49
1:B:86:ASN:ND2	1:B:86:ASN:H	2.10	0.49
1:B:295:VAL:HG11	1:B:438:MET:HE3	1.94	0.49
1:C:188:MET:HA	1:C:188:MET:HE2	1.93	0.49
1:A:22:ALA:HA	1:A:156:THR:HG23	1.95	0.48
1:C:61:HIS:HA	1:C:64:VAL:HG23	1.95	0.48
1:B:22:ALA:HA	1:B:156:THR:HG23	1.95	0.48
1:B:320:SER:O	1:B:323:ILE:HG22	2.13	0.48
1:C:126:ILE:HA	1:C:129:LEU:HD22	1.95	0.48
1:A:126:ILE:HA	1:A:129:LEU:HD22	1.95	0.48
1:B:391:GLY:HA2	1:B:485:MET:HB3	1.96	0.48
1:A:391:GLY:HA2	1:A:485:MET:HB3	1.96	0.48
1:C:391:GLY:HA2	1:C:485:MET:HB3	1.96	0.48
1:A:61:HIS:HA	1:A:64:VAL:HG23	1.96	0.48
1:C:314:LEU:HD12	1:C:383:THR:HB	1.96	0.48
1:A:314:LEU:HD12	1:A:383:THR:HB	1.96	0.47
1:B:314:LEU:HD12	1:B:383:THR:HB	1.96	0.47
1:A:320:SER:O	1:A:323:ILE:HG22	2.14	0.47
1:B:61:HIS:HA	1:B:64:VAL:HG23	1.96	0.47
1:A:336:GLU:HB2	1:A:339:MET:SD	2.55	0.47
1:C:320:SER:O	1:C:323:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:HB3	1:B:338:ALA:HB3	1.97	0.47
1:C:169:PRO:HB3	1:C:338:ALA:HB3	1.97	0.47
1:A:169:PRO:HB3	1:A:338:ALA:HB3	1.97	0.46
1:A:247:TYR:HB3	1:A:267:LEU:HD13	1.97	0.46
1:A:21:GLU:HG3	1:A:156:THR:HG21	1.97	0.46
1:C:312:TRP:CE3	1:C:450:VAL:HG13	2.51	0.46
1:C:247:TYR:HB3	1:C:267:LEU:HD13	1.98	0.46
1:A:88:ILE:HG22	1:A:126:ILE:HG12	1.98	0.46
1:A:312:TRP:CE3	1:A:450:VAL:HG13	2.50	0.45
1:B:336:GLU:HB2	1:B:339:MET:SD	2.56	0.45
1:B:21:GLU:HG3	1:B:156:THR:HG21	1.98	0.45
1:C:336:GLU:HB2	1:C:339:MET:SD	2.56	0.45
1:A:99:HIS:CE1	1:A:184:PRO:HB2	2.52	0.45
1:B:312:TRP:CE3	1:B:450:VAL:HG13	2.51	0.45
1:B:310:PRO:O	1:B:314:LEU:HG	2.17	0.45
1:C:21:GLU:HG3	1:C:156:THR:HG21	1.97	0.45
1:A:310:PRO:O	1:A:314:LEU:HG	2.17	0.45
1:C:310:PRO:O	1:C:314:LEU:HG	2.17	0.45
1:B:247:TYR:HB3	1:B:267:LEU:HD13	1.97	0.45
1:A:88:ILE:HA	1:A:126:ILE:HD11	1.98	0.44
1:B:371:THR:HB	1:B:374:ARG:HD2	1.99	0.44
1:C:39:LEU:HD13	1:C:56:ALA:HA	1.99	0.44
1:B:39:LEU:HD13	1:B:56:ALA:HA	1.98	0.44
1:C:371:THR:HB	1:C:374:ARG:HD2	2.00	0.44
1:A:289:ASP:C	1:A:291:ALA:H	2.25	0.44
1:B:14:ILE:N	1:B:15:PRO:CD	2.79	0.44
1:B:99:HIS:CE1	1:B:184:PRO:HB2	2.52	0.44
1:B:126:ILE:HA	1:B:129:LEU:HD22	1.99	0.44
1:C:289:ASP:C	1:C:291:ALA:H	2.26	0.44
1:A:39:LEU:HD13	1:A:56:ALA:HA	1.99	0.44
1:C:26:PHE:HB2	1:C:187:LEU:HD13	2.00	0.44
1:C:88:ILE:HG22	1:C:126:ILE:HG12	1.99	0.44
1:B:289:ASP:C	1:B:291:ALA:H	2.26	0.43
1:A:371:THR:HB	1:A:374:ARG:HD2	1.99	0.43
1:C:99:HIS:CE1	1:C:184:PRO:HB2	2.52	0.43
1:A:86:ASN:H	1:A:86:ASN:HD22	1.66	0.43
1:B:88:ILE:HG22	1:B:126:ILE:HG12	2.00	0.43
1:B:88:ILE:HA	1:B:126:ILE:HD11	2.00	0.43
1:B:154:TYR:HA	1:B:157:ILE:HD12	2.01	0.43
1:B:435:PRO:HG2	1:B:442:ILE:HD11	2.01	0.43
1:A:154:TYR:HA	1:A:157:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ILE:HA	1:C:126:ILE:HD11	2.01	0.43
1:C:154:TYR:HA	1:C:157:ILE:HD12	2.01	0.43
1:B:86:ASN:H	1:B:86:ASN:HD22	1.66	0.42
1:B:39:LEU:HD22	1:B:56:ALA:HA	2.01	0.42
1:B:439:LYS:C	1:B:441:THR:H	2.27	0.42
1:A:439:LYS:C	1:A:441:THR:H	2.27	0.42
1:A:26:PHE:HB2	1:A:187:LEU:HD13	2.01	0.42
1:B:305:PHE:CD1	1:B:446:TRP:HD1	2.37	0.42
1:C:86:ASN:H	1:C:86:ASN:HD22	1.66	0.42
1:C:305:PHE:CD1	1:C:446:TRP:HD1	2.37	0.42
1:A:39:LEU:HD22	1:A:56:ALA:HA	2.02	0.42
1:A:305:PHE:CD1	1:A:446:TRP:HD1	2.37	0.42
1:B:318:LYS:O	1:B:322:TRP:HB2	2.20	0.42
1:B:332:PRO:HD2	1:B:335:PHE:HB2	2.01	0.42
1:C:351:LEU:HD22	1:C:420:VAL:HG21	2.02	0.42
1:C:39:LEU:HD22	1:C:56:ALA:HA	2.02	0.42
1:A:332:PRO:HD2	1:A:335:PHE:HB2	2.01	0.41
1:C:301:ILE:HA	1:C:304:LEU:HD12	2.01	0.41
1:C:332:PRO:HD2	1:C:335:PHE:HB2	2.01	0.41
1:A:318:LYS:O	1:A:322:TRP:HB2	2.19	0.41
1:C:318:LYS:O	1:C:322:TRP:HB2	2.20	0.41
1:A:301:ILE:HA	1:A:304:LEU:HD12	2.01	0.41
1:A:388:ILE:HB	1:A:489:ALA:HB1	2.02	0.41
1:C:439:LYS:C	1:C:441:THR:H	2.27	0.41
1:B:26:PHE:HB2	1:B:187:LEU:HD13	2.02	0.41
1:B:301:ILE:HA	1:B:304:LEU:HD12	2.01	0.41
1:B:244:SER:HA	1:B:247:TYR:CD2	2.56	0.41
1:A:312:TRP:CE2	1:A:450:VAL:HG22	2.56	0.41
1:B:388:ILE:HB	1:B:489:ALA:HB1	2.02	0.41
1:C:312:TRP:CE2	1:C:450:VAL:HG22	2.55	0.41
1:C:313:SER:O	1:C:317:GLN:NE2	2.50	0.40
1:C:435:PRO:HG2	1:C:442:ILE:HD11	2.02	0.40
1:A:25:ARG:HD3	1:A:25:ARG:HA	1.95	0.40
1:A:244:SER:HA	1:A:247:TYR:CD2	2.56	0.40
1:A:435:PRO:HG2	1:A:442:ILE:HD11	2.03	0.40
1:C:35:LEU:O	1:C:39:LEU:HD12	2.22	0.40
1:B:299:LEU:HA	1:B:302:LEU:HD12	2.04	0.40
1:A:299:LEU:HA	1:A:302:LEU:HD12	2.04	0.40
1:B:312:TRP:CE2	1:B:450:VAL:HG22	2.56	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	449/524 (86%)	388 (86%)	55 (12%)	6 (1%)	9	37
1	B	449/524 (86%)	388 (86%)	55 (12%)	6 (1%)	9	37
1	C	449/524 (86%)	389 (87%)	54 (12%)	6 (1%)	9	37
All	All	1347/1572 (86%)	1165 (86%)	164 (12%)	18 (1%)	9	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	47	ILE
1	B	14	ILE
1	B	47	ILE
1	C	14	ILE
1	C	47	ILE
1	A	436	LYS
1	B	436	LYS
1	C	436	LYS
1	A	401	SER
1	A	403	LEU
1	B	401	SER
1	B	403	LEU
1	C	401	SER
1	C	403	LEU
1	A	440	GLY
1	C	440	GLY
1	B	440	GLY

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	367/427 (86%)	307 (84%)	60 (16%)	2	13
1	B	367/427 (86%)	306 (83%)	61 (17%)	2	13
1	C	367/427 (86%)	306 (83%)	61 (17%)	2	13
All	All	1101/1281 (86%)	919 (84%)	182 (16%)	2	13

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	36	THR
1	A	39	LEU
1	A	45	LEU
1	A	47	ILE
1	A	50	GLU
1	A	52	ARG
1	A	64	VAL
1	A	65	ILE
1	A	73	LEU
1	A	85	TYR
1	A	86	ASN
1	A	87	THR
1	A	92	SER
1	A	93	LEU
1	A	97	VAL
1	A	121	LEU
1	A	126	ILE
1	A	130	VAL
1	A	166	LEU
1	A	167	SER
1	A	171	LEU
1	A	179	VAL
1	A	183	ILE
1	A	193	VAL
1	A	197	LEU
1	A	203	ILE
1	A	235	LEU
1	A	237	LEU
1	A	257	ILE
1	A	284	ARG

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Mol	Chain	Res	Type
1	A	289	ASP
1	A	293	ASP
1	A	299	LEU
1	A	308	VAL
1	A	309	THR
1	A	324	LEU
1	A	325	GLN
1	A	328	ASP
1	A	347	LEU
1	A	351	LEU
1	A	380	ILE
1	A	390	VAL
1	A	394	GLN
1	A	396	MET
1	A	405	ILE
1	A	412	TYR
1	A	414	LEU
1	A	415	LEU
1	A	416	THR
1	A	447	THR
1	A	448	LEU
1	A	451	THR
1	A	455	LEU
1	A	458	LEU
1	A	464	VAL
1	A	480	VAL
1	A	481	THR
1	A	491	PHE
1	A	499	PHE
1	B	35	LEU
1	B	36	THR
1	B	39	LEU
1	B	45	LEU
1	B	47	ILE
1	B	50	GLU
1	B	52	ARG
1	B	64	VAL
1	B	65	ILE
1	B	73	LEU
1	B	85	TYR
1	B	86	ASN
1	B	87	THR

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Mol	Chain	Res	Type
1	B	92	SER
1	B	93	LEU
1	B	97	VAL
1	B	121	LEU
1	B	126	ILE
1	B	130	VAL
1	B	166	LEU
1	B	167	SER
1	B	171	LEU
1	B	179	VAL
1	B	183	ILE
1	B	193	VAL
1	B	197	LEU
1	B	203	ILE
1	B	235	LEU
1	B	237	LEU
1	B	257	ILE
1	B	284	ARG
1	B	289	ASP
1	B	293	ASP
1	B	299	LEU
1	B	308	VAL
1	B	309	THR
1	B	324	LEU
1	B	325	GLN
1	B	328	ASP
1	B	347	LEU
1	B	351	LEU
1	B	380	ILE
1	B	390	VAL
1	B	394	GLN
1	B	396	MET
1	B	405	ILE
1	B	412	TYR
1	B	414	LEU
1	B	415	LEU
1	B	416	THR
1	B	447	THR
1	B	448	LEU
1	B	451	THR
1	B	455	LEU
1	B	458	LEU

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Mol	Chain	Res	Type
1	B	464	VAL
1	B	480	VAL
1	B	481	THR
1	B	485	MET
1	B	491	PHE
1	B	499	PHE
1	C	35	LEU
1	C	36	THR
1	C	39	LEU
1	C	45	LEU
1	C	47	ILE
1	C	50	GLU
1	C	52	ARG
1	C	64	VAL
1	C	65	ILE
1	C	73	LEU
1	C	85	TYR
1	C	86	ASN
1	C	87	THR
1	C	92	SER
1	C	93	LEU
1	C	97	VAL
1	C	121	LEU
1	C	126	ILE
1	C	130	VAL
1	C	166	LEU
1	C	167	SER
1	C	171	LEU
1	C	179	VAL
1	C	183	ILE
1	C	193	VAL
1	C	197	LEU
1	C	203	ILE
1	C	235	LEU
1	C	237	LEU
1	C	257	ILE
1	C	284	ARG
1	C	289	ASP
1	C	293	ASP
1	C	299	LEU
1	C	308	VAL
1	C	309	THR

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Mol	Chain	Res	Type
1	C	324	LEU
1	C	325	GLN
1	C	328	ASP
1	C	347	LEU
1	C	351	LEU
1	C	380	ILE
1	C	390	VAL
1	C	394	GLN
1	C	396	MET
1	C	405	ILE
1	C	412	TYR
1	C	414	LEU
1	C	415	LEU
1	C	416	THR
1	C	447	THR
1	C	448	LEU
1	C	451	THR
1	C	455	LEU
1	C	458	LEU
1	C	464	VAL
1	C	480	VAL
1	C	481	THR
1	C	485	MET
1	C	491	PHE
1	C	499	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	158	ASN
1	A	251	ASN
1	A	355	ASN
1	A	356	ASN
1	B	142	ASN
1	B	158	ASN
1	B	251	ASN
1	B	355	ASN
1	C	142	ASN
1	C	158	ASN
1	C	251	ASN
1	C	355	ASN

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Mol	Chain	Res	Type
1	C	356	ASN
1	C	454	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	371:THR	C	372:ALA	N	3.72
1	B	371:THR	C	372:ALA	N	3.72
1	C	371:THR	C	372:ALA	N	3.72

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	456/524 (87%)	-0.15	0 100 100	77, 270, 300, 300	0
1	B	456/524 (87%)	-0.06	3 (0%) 84 62	78, 280, 300, 300	0
1	C	456/524 (87%)	-0.00	7 (1%) 72 46	87, 290, 300, 300	0
All	All	1368/1572 (87%)	-0.07	10 (0%) 84 62	77, 282, 300, 300	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	379	GLY	3.4
1	C	283	ALA	3.3
1	B	273	GLY	3.1
1	C	381	ALA	3.0
1	C	372	ALA	2.6
1	C	306	ALA	2.5
1	C	139	ASP	2.3
1	B	274	ALA	2.1
1	B	437	ALA	2.1
1	C	254	THR	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.