



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:24 AM UTC

PDB ID : 7QYG / pdb_00007qyg
Title : Structure of the transaminase TR2
Authors : Roda, S.; Fernandez-Lopez, L.; Benedens, M.; Bollinger, A.; Thies, S.; Schumacher, J.; Coscolin, C.; Kazemi, M.; Santiago, G.; Gertzen, C.G.; Gonzalez-Alfonso, J.; Plou, F.J.; Jaeger, K.E.; Smits, S.H.; Ferrer, M.; Guallar, V.
Deposited on : 2022-01-28
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

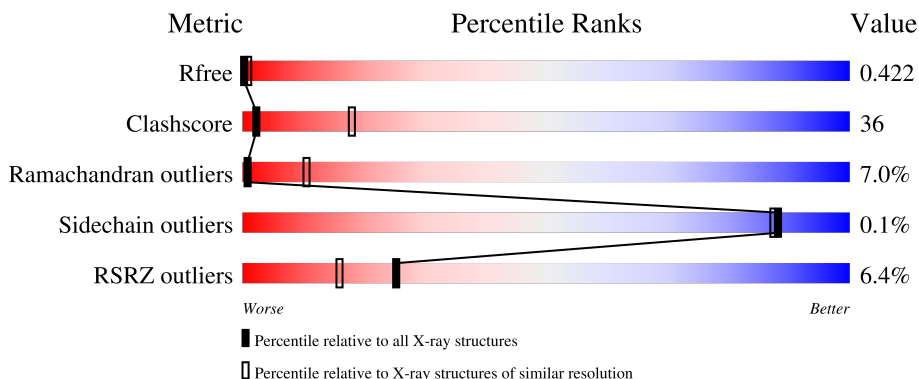
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	465	5% 32% 48% 16%
1	B	465	5% 38% 42% 16%
1	C	465	8% 34% 46% 5% 16%
1	D	465	4% 37% 43% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24079 atoms, of which 12003 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 Aminotransferase TR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	389	Total	C	H	N	O	S	0	0	0
			6017	1917	3000	525	558	17			
1	B	389	Total	C	H	N	O	S	0	0	0
			6005	1914	2992	524	558	17			
1	C	391	Total	C	H	N	O	S	0	0	0
			6052	1926	3019	530	560	17			
1	D	389	Total	C	H	N	O	S	0	0	0
			6005	1914	2992	524	558	17			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	458	LEU	-	expression tag	UNP A0A3G5BC54
A	459	GLU	-	expression tag	UNP A0A3G5BC54
A	460	HIS	-	expression tag	UNP A0A3G5BC54
A	461	HIS	-	expression tag	UNP A0A3G5BC54
A	462	HIS	-	expression tag	UNP A0A3G5BC54
A	463	HIS	-	expression tag	UNP A0A3G5BC54
A	464	HIS	-	expression tag	UNP A0A3G5BC54
A	465	HIS	-	expression tag	UNP A0A3G5BC54
B	458	LEU	-	expression tag	UNP A0A3G5BC54
B	459	GLU	-	expression tag	UNP A0A3G5BC54
B	460	HIS	-	expression tag	UNP A0A3G5BC54
B	461	HIS	-	expression tag	UNP A0A3G5BC54
B	462	HIS	-	expression tag	UNP A0A3G5BC54
B	463	HIS	-	expression tag	UNP A0A3G5BC54
B	464	HIS	-	expression tag	UNP A0A3G5BC54
B	465	HIS	-	expression tag	UNP A0A3G5BC54
C	458	LEU	-	expression tag	UNP A0A3G5BC54
C	459	GLU	-	expression tag	UNP A0A3G5BC54
C	460	HIS	-	expression tag	UNP A0A3G5BC54
C	461	HIS	-	expression tag	UNP A0A3G5BC54
C	462	HIS	-	expression tag	UNP A0A3G5BC54

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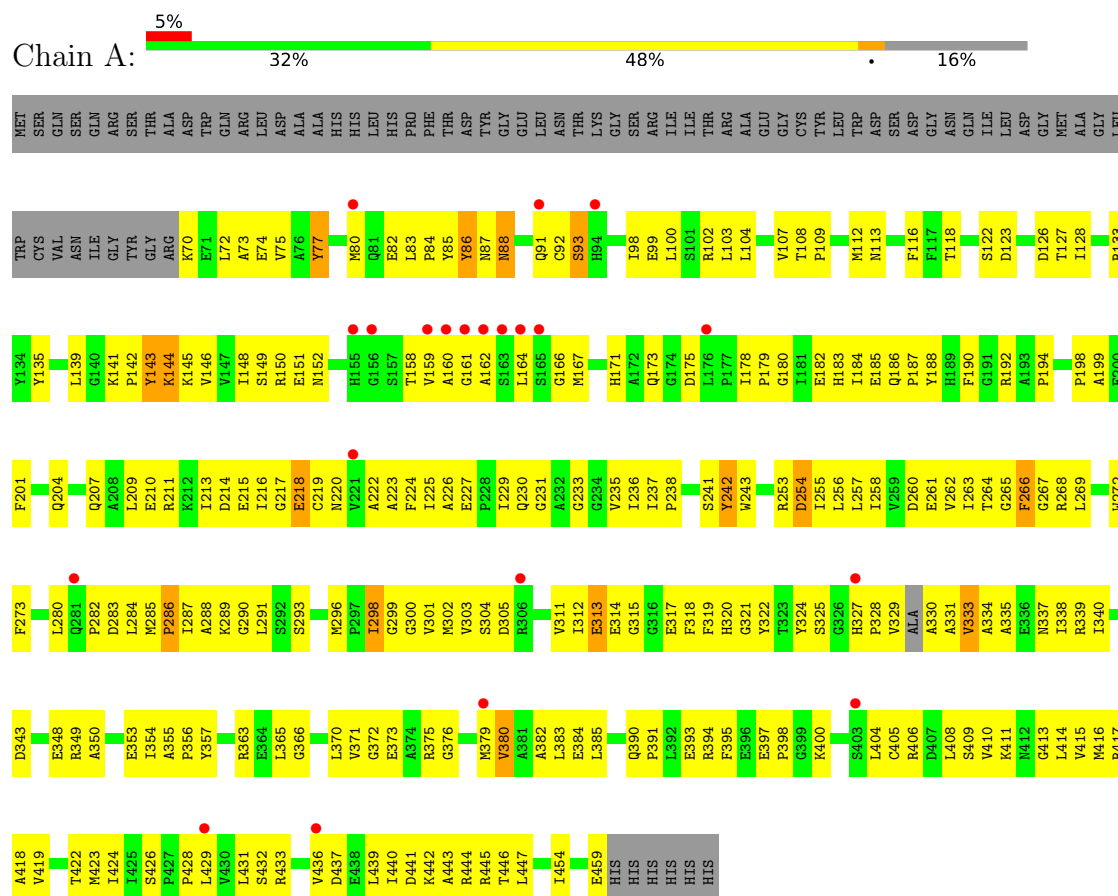
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Chain	Residue	Modelled	Actual	Comment	Reference
C	463	HIS	-	expression tag	UNP A0A3G5BC54
C	464	HIS	-	expression tag	UNP A0A3G5BC54
C	465	HIS	-	expression tag	UNP A0A3G5BC54
D	458	LEU	-	expression tag	UNP A0A3G5BC54
D	459	GLU	-	expression tag	UNP A0A3G5BC54
D	460	HIS	-	expression tag	UNP A0A3G5BC54
D	461	HIS	-	expression tag	UNP A0A3G5BC54
D	462	HIS	-	expression tag	UNP A0A3G5BC54
D	463	HIS	-	expression tag	UNP A0A3G5BC54
D	464	HIS	-	expression tag	UNP A0A3G5BC54
D	465	HIS	-	expression tag	UNP A0A3G5BC54

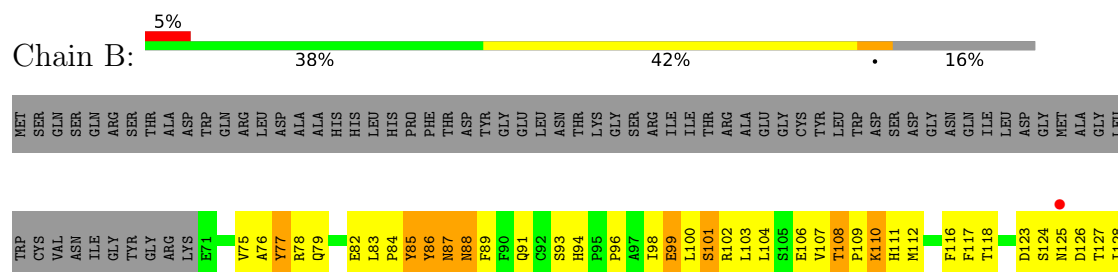
3 Residue-property plots

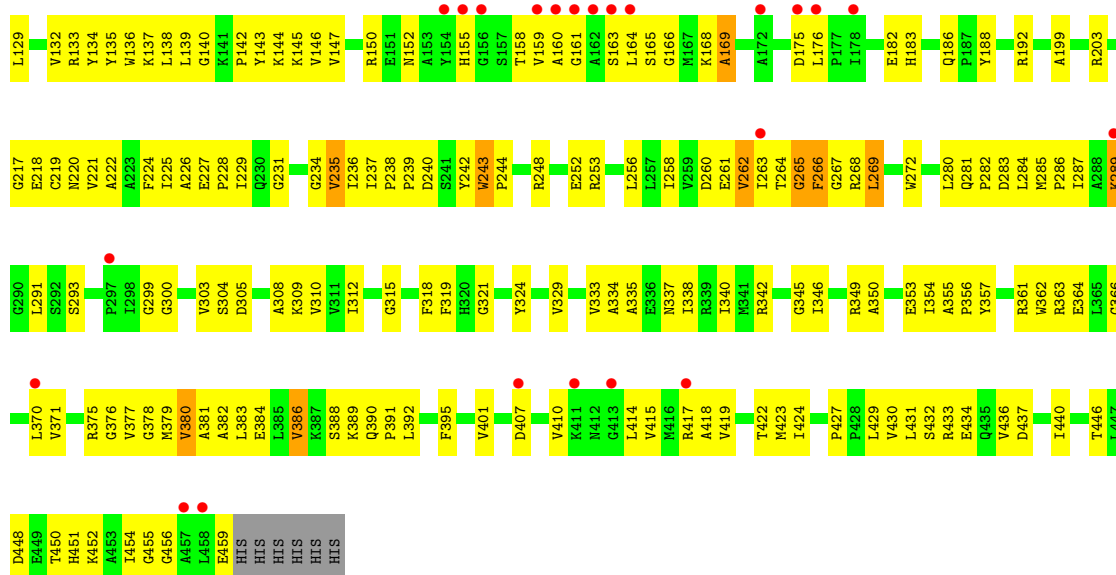
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aminotransferase TR2

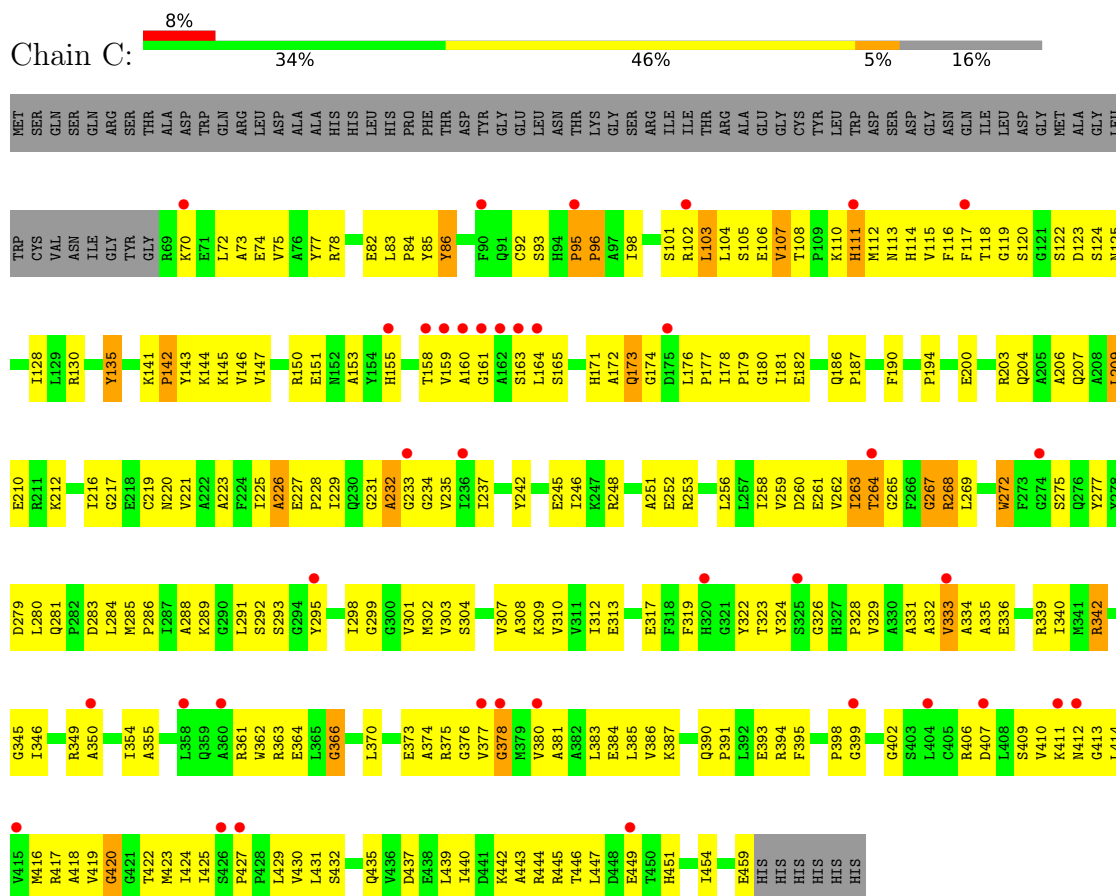


• Molecule 1: Aminotransferase TR2

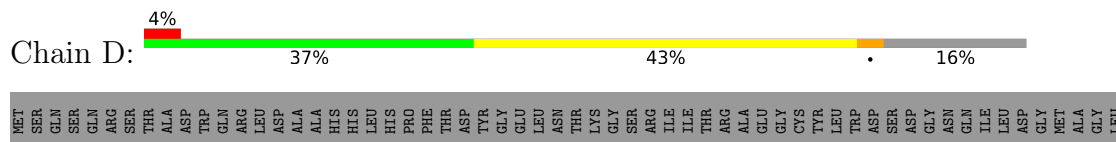




• Molecule 1: Aminotransferase TR2



• Molecule 1: Aminotransferase TR2



R444	R445	T446	L447	D448	I454	E459	H1S	H1S	H1S	H1S	H1S	H1S	K141	P142	Y143	K144	K145	I146	GLY	TYR	GLY	ARG	LYS	E71	V75	A76	Y77	L83	P84	Y85	Y86	N87	N88	F89	F90	Q91	H94	P95	P96	A97	I98	E99	L100	S101	R102	L103	L104	S105	E106	V107	T108	P109	K110	H111	M112	M113	D126	T127	T128	L129	R130	Y134	Y135	W136	K137	L138	L139	G140
G299	G300	V301	M302	V303	S304	D305	R306	V307	A308	K309	V310	V311	I312	G315	G316	E317	F318	F319	Y322	A332	V333	A334	A335	E336	N337	I338	R339	I340	P341	R342	D343	E344	G345	I346	I347	E348	R349	A350	I354	A355	P356	Y357	L358	L365	G366	E367	H368	P369	L370	V371	G372	A373	R375															
K379	V380	A381	A382	L383	E384	L385	V386	K387	S388	K389	Q390	P391	R394	F395	G399	K400	V401	G402	S403	L404	C405	R406	D407	V410	K411	N412	G413	L414	V415	M416	G420	G421	T422	M423	I424	I425	S426	P427	P428	L429	V430	L431	S432	R433	E434	Q435	V436	D437	E438	L439	I440	D441	K442	A443														
A222	A223	F224	I225	A226	E227	P228	I229	Q230	G231	A232	I236	I237	P238	P239	Y242	I243	F244	E245	I246	K247	R248	R253	L256	I257	I258	V259	I260	E261	V262	I263	T264	G265	F266	G267	R268	L269	Q272	F273	G274	S275	Q276	L280	Q281	P282	D283	L284	M285	P286	I287	A288	K289	G290																
K141	P142	Y143	K144	K145	I146	GLY	TYR	GLY	ARG	LYS	E71	V75	A76	Y77	L83	P84	Y85	Y86	N87	N88	F89	F90	Q91	H94	P95	P96	A97	I98	E99	L100	S101	R102	L103	L104	S105	E106	V107	T108	P109	K110	H111	M112	M113	D126	T127	T128	L129	R130	Y134	Y135	W136	K137	L138	L139	G140													

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.78Å 166.63Å 209.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 3.60 49.09 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.09-3.60) 94.2 (49.09-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.345 , 0.422 0.346 , 0.422	Depositor DCC
R_{free} test set	2000 reflections (7.82%)	wwPDB-VP
Wilson B-factor (Å ²)	113.7	Xtriage
Anisotropy	0.935	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	24079	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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](#)

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	0.29	0/3086	0.54	0/4176
1	B	0.31	0/3082	0.57	0/4172
1	C	0.35	1/3102 (0.0%)	0.60	0/4197
1	D	0.36	0/3082	0.58	1/4172 (0.0%)
All	All	0.33	1/12352 (0.0%)	0.57	1/16717 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	435	GLN	CA-C	5.23	1.61	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	MET	CG-SD-CE	5.43	112.84	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Peptide

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	3017	3000	3000	218	0
1	B	3013	2992	2992	207	0
1	C	3033	3019	3018	239	0
1	D	3013	2992	2992	228	0
All	All	12076	12003	12002	873	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 36.

The worst 5 of 873 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:128:ILE:HD13	1:B:258:ILE:CD1	1.66	1.25
1:B:128:ILE:HD13	1:B:258:ILE:HD11	1.15	1.09
1:D:347:ILE:HD11	1:D:348:GLU:OE2	1.51	1.09
1:D:347:ILE:CD1	1:D:348:GLU:OE2	2.03	1.06
1:B:128:ILE:CD1	1:B:258:ILE:CD1	2.35	1.05

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	387/465 (83%)	287 (74%)	75 (19%)	25 (6%)	1 12
1	B	387/465 (83%)	285 (74%)	71 (18%)	31 (8%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	389/465 (84%)	272 (70%)	87 (22%)	30 (8%)	1	9
1	D	387/465 (83%)	287 (74%)	78 (20%)	22 (6%)	1	13
All	All	1550/1860 (83%)	1131 (73%)	311 (20%)	108 (7%)	1	10

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	GLU
1	B	101	SER
1	B	236	ILE
1	B	243	TRP
1	B	266	PHE

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	315/377 (84%)	315 (100%)	0	100	100
1	B	314/377 (83%)	314 (100%)	0	100	100
1	C	316/377 (84%)	315 (100%)	1 (0%)	86	83
1	D	314/377 (83%)	314 (100%)	0	100	100
All	All	1259/1508 (84%)	1258 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	337	ASN

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Mol	Chain	Res	Type
1	D	368	HIS
1	D	155	HIS
1	B	276	GLN
1	C	220	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](#)

There are no chain breaks in this entry.

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	389/465 (83%)	0.30	21 (5%)	31	18	84, 136, 185, 222	0
1	B	389/465 (83%)	0.31	24 (6%)	26	16	89, 131, 177, 225	0
1	C	391/465 (84%)	0.66	38 (9%)	13	10	88, 152, 189, 223	0
1	D	389/465 (83%)	0.42	17 (4%)	39	22	90, 146, 200, 225	0
All	All	1558/1860 (83%)	0.42	100 (6%)	25	16	84, 140, 191, 225	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	SER	8.0
1	B	175	ASP	5.8
1	C	102	ARG	5.5
1	B	164	LEU	5.3
1	D	175	ASP	5.2

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.