



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:52 PM UTC

PDB ID : 3PJZ / pdb_00003pjz
Title : Crystal Structure of the Potassium Transporter TrkH from *Vibrio parahaemolyticus*
Authors : Cao, Y.; Jin, X.; Huang, H.; Levin, E.J.; Zhou, M.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : 2010-11-10
Resolution : 3.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

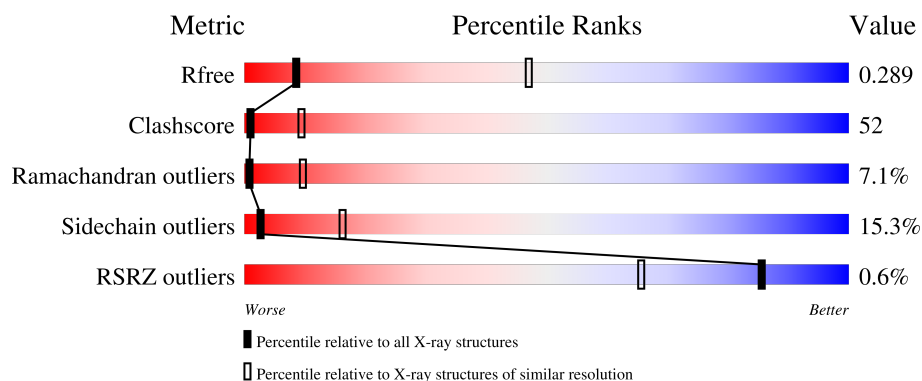
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	494	31% 48% 15% • 5%
1	B	494	30% 50% 14% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7242 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 Potassium uptake protein TrkH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3620	2421	574	607	18			
1	B	468	Total	C	N	O	S	0	0	0
			3620	2421	574	607	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	ALA	-	expression tag	UNP Q87TN7
A	487	ALA	-	expression tag	UNP Q87TN7
A	488	ALA	-	expression tag	UNP Q87TN7
A	489	GLU	-	expression tag	UNP Q87TN7
A	490	ASN	-	expression tag	UNP Q87TN7
A	491	LEU	-	expression tag	UNP Q87TN7
A	492	TYR	-	expression tag	UNP Q87TN7
A	493	PHE	-	expression tag	UNP Q87TN7
A	494	GLN	-	expression tag	UNP Q87TN7
B	486	ALA	-	expression tag	UNP Q87TN7
B	487	ALA	-	expression tag	UNP Q87TN7
B	488	ALA	-	expression tag	UNP Q87TN7
B	489	GLU	-	expression tag	UNP Q87TN7
B	490	ASN	-	expression tag	UNP Q87TN7
B	491	LEU	-	expression tag	UNP Q87TN7
B	492	TYR	-	expression tag	UNP Q87TN7
B	493	PHE	-	expression tag	UNP Q87TN7
B	494	GLN	-	expression tag	UNP Q87TN7

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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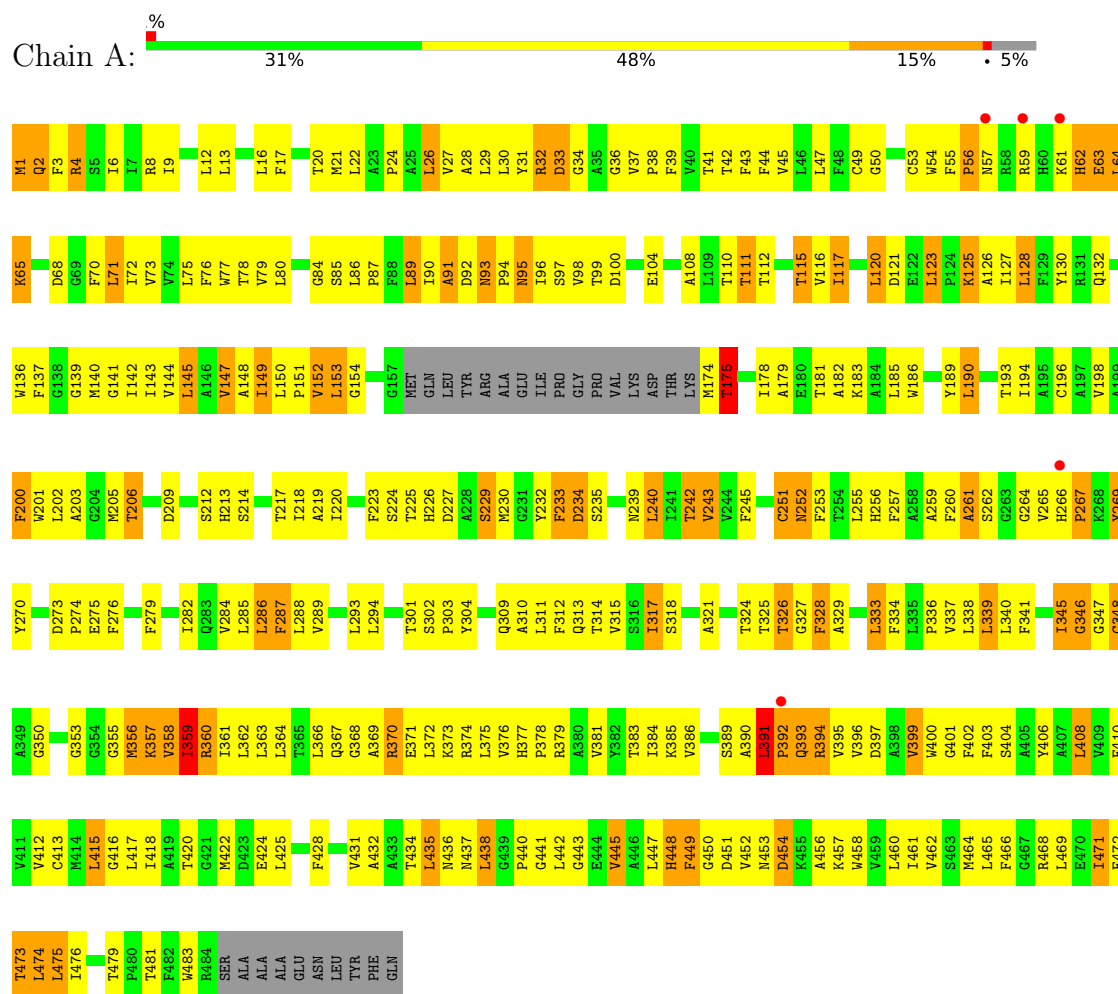
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		

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: Potassium uptake protein TrkH



• Molecule 1: Potassium uptake protein TrkH



L64	K65	S66	R67	D68	F69	L70	L71	I72	V73	V74	L75	F76	W77	V78	V79	L80	G84	S85	L86	P87	F88	L89	I90	A91	D92	N93	P94	N95	I96	S97	V98	T99	D100	E104	A108	L109	T110	T111	T115	V116	I117	L120	D121	E122	L123	K125	A126	I127	L128	F129	Y130	R131	Q132			
F133	L134	Q135	W136	F137	G138	G139	M140	G141	I142	I143	V144	L145	A146	V147	A148	I149	L150	P151	V152	L153	G154	G157	MET	GLN	LEU	TYR	ARG	ALA	GLU	ILE	PRO	GLY	PRO	VAL	LYS	ASP	THR	LYS	M174	T175	I178	A179	E180	T181	A182	K183	A184	L185	W186	F260	Y189	L190	T193	I194	A195	C196
A197	V198	A199	F200	W201	L202	A203	G204	M205	T206	D209	S212	H213	S214	T217	I218	A219	I220	F223	S224	T225	H226	D227	A228	S229	M230	G231	Y232	F233	D234	S235	N239	L240	T241	T242	V243	V244	F245	C251	N252	L255	H256	F257	A258	A259	F260	A261	S262	G263	G264	V265	P267					
K268	Y269	Y270	D273	G416	P274	E275	F276	F279	I282	G283	V284	L285	L286	L287	L288	V289	C290	L293	L294	T301	S302	P303	Y304	Q309	A310	L311	F312	Q313	T314	V315	S316	I317	S318	A321	T324	T325	T326	G327	F328	A329	L333	F334	L335	P336	V337	L338	L339	L340	F341	I345						
G346	G347	C348	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411		
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366	L366	Q367	G368	A369	R370	E371	L372	K373	R374	L375	V376	H377	P378	T383	I384	K385	V386	S389	A390	L391	P392	Q393	R394	V395	V396	D397	A398	V399	W400	G401	F402	F403	S404	A405	Y406	A407	L408	V409	V411	
V412	C413	M414	L415	A349	G350	G353	M356	K357	V358	L359	R360	I361	L362	L363	L364	T366																																								

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.49Å 97.41Å 195.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.51 14.99 – 3.51	Depositor EDS
% Data completeness (in resolution range)	85.7 (14.99-3.51) 84.4 (14.99-3.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	18.32 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.249 , 0.299 0.243 , 0.289	Depositor DCC
R_{free} test set	1008 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7242	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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	0.57	0/3723	0.95	10/5073 (0.2%)
1	B	0.54	0/3723	0.94	9/5073 (0.2%)
All	All	0.56	0/7446	0.95	19/10146 (0.2%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	LEU	CA-C-N	9.48	131.69	119.84
1	B	391	LEU	C-N-CA	9.48	131.69	119.84
1	A	391	LEU	CA-C-N	9.10	131.21	119.84
1	A	391	LEU	C-N-CA	9.10	131.21	119.84
1	B	251	CYS	N-CA-C	7.84	121.43	108.49

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	3620	0	3696	394	0
1	B	3620	0	3696	395	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7242	0	7392	764	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 52.

The worst 5 of 764 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:A:136:TRP:HE1	1:A:193:THR:HG21	0.97	1.12
1:B:136:TRP:HE1	1:B:193:THR:HG21	0.95	1.06
1:B:93:ASN:HB2	1:B:94:PRO:HD3	1.40	1.04
1:B:132:GLN:HG3	1:B:212:SER:HB2	1.38	1.04
1:A:93:ASN:HB2	1:A:94:PRO:HD3	1.41	1.00

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	464/494 (94%)	337 (73%)	93 (20%)	34 (7%)	1	9
1	B	464/494 (94%)	338 (73%)	94 (20%)	32 (7%)	1	10
All	All	928/988 (94%)	675 (73%)	187 (20%)	66 (7%)	1	10

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	91	ALA
1	A	175	THR
1	A	267	PRO

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Mol	Chain	Res	Type
1	A	329	ALA

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	380/401 (95%)	322 (85%)	58 (15%)	3	16
1	B	380/401 (95%)	322 (85%)	58 (15%)	3	16
All	All	760/802 (95%)	644 (85%)	116 (15%)	3	16

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	481	THR
1	B	454	ASP
1	B	117	ILE
1	B	448	HIS
1	B	383	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	ASN
1	B	252	ASN
1	B	226	HIS
1	B	256	HIS
1	A	256	HIS

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](#)

Of 2 ligands modelled in this entry, 2 are 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 [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	468/494 (94%)	-0.16	5 (1%)	78 54	17, 53, 112, 179	0
1	B	468/494 (94%)	-0.17	1 (0%)	91 82	18, 53, 115, 178	0
All	All	936/988 (94%)	-0.17	6 (0%)	85 65	17, 53, 113, 179	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	HIS	3.2
1	A	57	ASN	2.8
1	B	392	PRO	2.5
1	A	61	LYS	2.5
1	A	59	ARG	2.4

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($\text{\AA}^2$)	Q<0.9
2	K	A	501	1/1	0.97	0.06	41,41,41,41	0
2	K	B	501	1/1	0.99	0.06	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.