



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:20 AM UTC

PDB ID : 1DTQ / pdb_00001dtq
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH PETT-1 (PETT131A94)
Authors : Ren, J.; Diprose, J.; Warren, J.; Esnouf, R.M.; Bird, L.E.; Ikemizu, S.; Slater,
M.; Milton, J.; Balzarini, J.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2000-01-13
Resolution : 2.80 Å(reported)

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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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

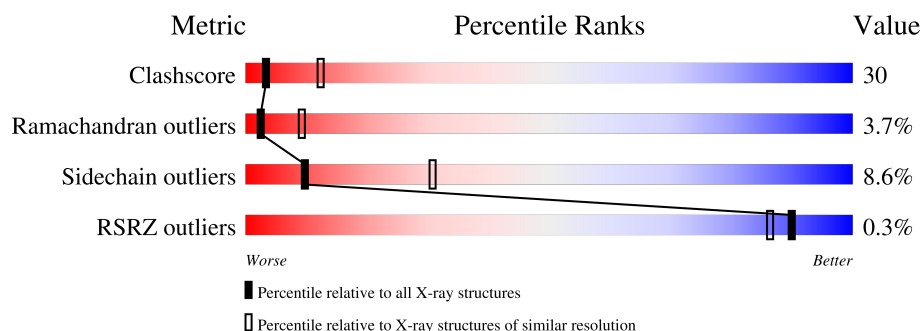
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	560	
2	B	440	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSD	A	280	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7687 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.

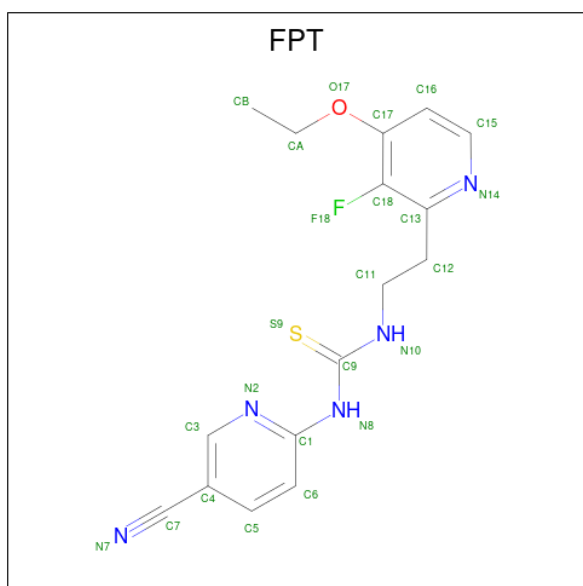
- Molecule 1 is a protein called HIV-1 RT A-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4310	2792	714	796	8			

- Molecule 2 is a protein called HIV-1 RT B-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3327	2166	550	605	6			

- Molecule 3 is N-[[3-FLUORO-4-ETHOXY-PYRID-2-YL]ETHYL]-N'-[5-NITRILOMETHYL-PYRIDYL]-THIOUREA (CCD ID: FPT) (formula: C₁₆H₁₆FN₅OS).

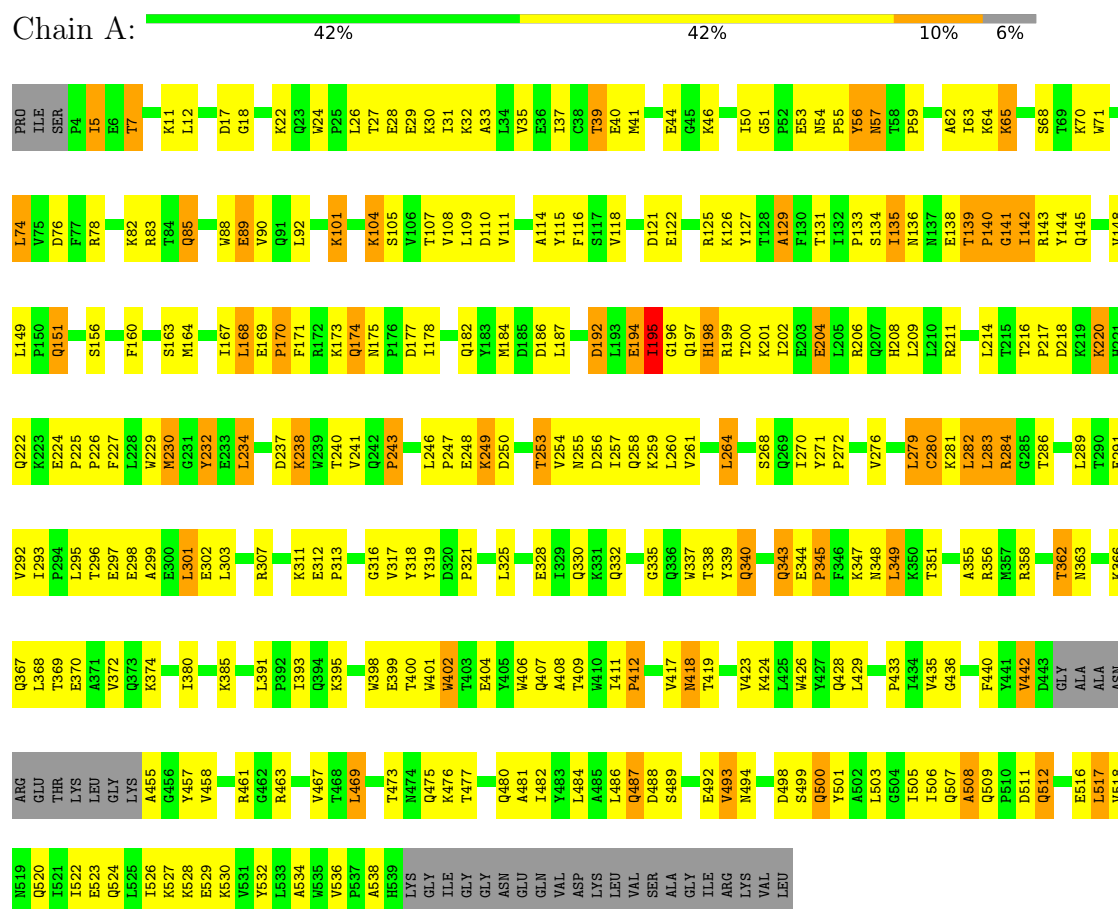


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	8	Total 8	O 8	0	0

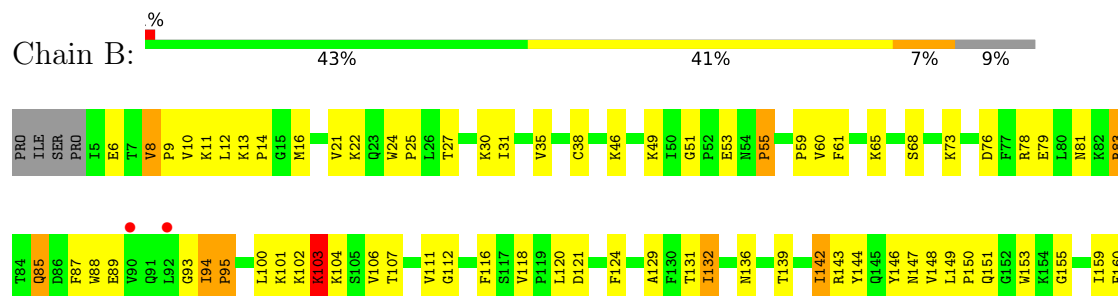
3 Residue-property plots

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: HIV-1 RT A-CHAIN



• Molecule 2: HIV-1 RT B-CHAIN



T377	A299	Q161	PRO	G231	K166	L167	R172	K173	Q174	N175	P176	D177	I178	V179	Y183	M184	D185	V189	G190	S191	D192	L193	E194	I195	G196	Q197	H198	R199	T200	K201	L202	E203	E204	L205	R206	Q207	H208	L209	L210	R211	W212	G213	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU
E378	E300	S162	PRO	Y232	T165	L168	F171	R173	Q174	N175	P176	D177	I178	V179	Y183	M184	D185	V189	G190	S191	D192	L193	E194	I195	G196	Q197	H198	R199	T200	K201	L202	E203	E204	L205	R206	Q207	H208	L209	L210	R211	W212	G213	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU
S379	E301	S163	PHE	E233	T166	L169	F172	K174	Q175	N176	P177	D178	I179	V180	Y184	M185	D186	V190	G191	S192	D193	L194	E195	I196	G197	Q198	H199	R200	K202	L203	E204	L206	R207	Q208	H209	L211	R212	W213	G214	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU			
I382	E302	S164	LEU	E234	T167	L170	F173	K175	Q176	N177	P178	D179	I180	V181	Y185	M186	D187	V191	G192	S193	D194	L195	E196	I197	G198	Q199	H200	R201	K203	L204	E205	L207	Q209	H210	L212	R213	W214	G215	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
V383	E303	S165	TRP	E235	T168	L171	F174	K176	Q177	N178	P179	D180	I181	V182	Y186	M187	D188	V192	G193	S194	D195	L196	E197	I198	G199	Q200	H201	R202	K204	L205	E206	L208	Q210	H211	L213	R214	W215	G216	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
G384	E304	S166	MET	E236	T169	L172	F175	K177	Q178	N179	P180	D181	I182	V183	Y187	M188	D189	V193	G194	S195	D196	L197	E198	I199	G200	Q201	H202	R203	K205	L206	E207	L209	Q211	H212	L214	R215	W216	G217	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
K385	E305	S167	LEU	E237	T170	L173	F176	K178	Q179	N180	P181	D182	I183	V184	Y188	M189	D190	V194	G195	S196	D197	L198	E199	I200	G201	Q202	H203	R204	K206	L207	E208	L210	Q212	H213	L215	R216	W217	G218	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
T386	E306	S168	TRP	E238	T171	L174	F177	K179	Q180	N181	P182	D183	I184	V185	Y189	M190	D191	V195	G196	S197	D198	L199	E200	I201	G202	Q203	H204	R205	K207	L208	E209	L211	Q213	H214	L216	R217	W218	G219	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
P387	E307	S169	LEU	E239	T172	L175	F178	K180	Q181	N182	P183	D184	I185	V186	Y190	M191	D192	V196	G197	S198	D199	L200	E201	I202	G203	Q204	H205	R206	K208	L209	E210	L212	Q214	H215	L217	R218	W219	G220	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
K388	E308	S170	TRP	E240	T173	L176	F179	K181	Q182	N183	P184	D185	I186	V187	Y191	M192	D193	V197	G198	S199	D200	L201	E202	I203	G204	Q205	H206	R207	K209	L210	E211	L213	Q215	H216	L218	R219	W220	G221	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
F389	E309	S171	LEU	E241	T174	L177	F180	K182	Q183	N184	P185	D186	I187	V188	Y192	M193	D194	V198	G199	S200	D201	L202	E203	I204	G205	Q206	H207	R208	K210	L211	E212	L214	Q216	H217	L219	R220	W221	G222	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
I393	E310	S172	TRP	E242	T175	L178	F181	K183	Q184	N185	P186	D187	I188	V189	Y193	M194	D195	V199	G200	S201	D202	L203	E204	I205	G206	Q207	H208	R209	K211	L212	E213	L215	Q217	H218	L220	R221	W222	G223	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
Q394	E311	S173	LEU	E243	T176	L179	F182	K184	Q185	N186	P187	D188	I189	V190	Y194	M195	D196	V200	G201	S202	D203	L204	E205	I206	G207	Q208	H209	R210	K212	L213	E214	L216	Q218	H219	L221	R222	W223	G224	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
K395	E312	S174	TRP	E244	T177	L180	F183	K185	Q186	N187	P188	D189	I190	V191	Y195	M196	D197	V201	G202	S203	D204	L205	E206	I207	G208	Q209	H210	R211	K213	L214	E215	L217	Q219	H220	L222	R223	W224	G225	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
V398	E313	S175	LEU	E245	T178	L181	F184	K186	Q187	N188	P189	D190	I191	V192	Y196	M197	D198	V202	G203	S204	D205	L206	E207	I208	G209	Q210	H211	R212	K214	L215	E216	L218	Q220	H221	L223	R224	W225	G226	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
W401	E314	S176	TRP	E246	T179	L182	F185	K187	Q188	N189	P190	D191	I192	V193	Y197	M198	D199	V203	G204	S205	D206	L207	E208	I209	G210	Q211	H212	R213	K215	L216	E217	L219	Q221	H222	L224	R225	W226	G227	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
W402	E315	S177	LEU	E247	T180	L183	F186	K188	Q189	N190	P191	D192	I193	V194	Y198	M199	D200	V204	G205	S206	D207	L208	E209	I210	G211	Q212	H213	R214	K216	L217	E218	L220	Q222	H223	L225	R226	W227	G228	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
T403	E316	S178	TRP	E248	T181	L184	F187	K189	Q190	N191	P192	D193	I194	V195	Y199	M200	D201	V205	G206	S207	D208	L209	E210	I211	G212	Q213	H214	R215	K217	L218	E219	L221	Q223	H224	L226	R227	W228	G229	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
E404	E317	S179	LEU	E249	T182	L185	F188	K190	Q191	N192	P193	D194	I195	V196	Y200	M201	D202	V206	G207	S208	D209	L210	E211	I212	G213	Q214	H215	R216	K218	L219	E220	L222	Q224	H225	L227	R228	W229	G230	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
Y405	E318	S180	TRP	E250	T183	L186	F189	K191	Q192	N193	P194	D195	I196	V197	Y201	M202	D203	V207	G208	S209	D210	L211	E212	I213	G214	Q215	H216	R217	K219	L220	E221	L223	Q225	H226	L228	R229	W230	G231	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
W406	E319	S181	LEU	E251	T184	L187	F190	K192	Q193	N194	P195	D196	I197	V198	Y202	M203	D204	V208	G209	S210	D211	L212	E213	I214	G215	Q216	H217	R218	K220	L221	E222	L224	Q226	H227	L229	R230	W231	G232	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
I418	E320	S182	TRP	E252	T185	L188	F191	K193	Q194	N195	P196	D197	I198	V199	Y203	M204	D205	V209	G210	S211	D212	L213	E214	I215	G216	Q217	H218	R219	K221	L222	E223	L225	Q227	H228	L230	R231	W232	G233	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
T419	E321	S183	LEU	E253	T186	L189	F192	K194	Q195	N196	P197	D198	I199	V200	Y204	M205	D206	V210	G211	S212	D213	L214	E215	I216	G217	Q218	H219	R220	K222	L223	E224	L226	Q228	H229	L231	R232	W233	G234	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
P420	E322	S184	TRP	E254	T187	L190	F193	K195	Q196	N197	P198	D199	I200	V201	Y205	M206	D207	V211	G212	S213	D214	L215	E216	I217	G218	Q219	H220	R221	K223	L224	E225	L227	Q229	H230	L232	R233	W234	G235	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
P421	E323	S185	LEU	E255	T188	L191	F194	K196	Q197	N198	P199	D200	I201	V202	Y206	M207	D208	V212	G213	S214	D215	L216	E217	I218	G219	Q220	H221	R222	K224	L225	E226	L228	Q230	H231	L233	R234	W235	G236	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
L422	E324	S186	TRP	E256	T189	L192	F195	K197	Q198	N199	P200	D201	I202	V203	Y207	M208	D209	V213	G214	S215	D216	L217	E218	I219	G220	Q221	H222	R223	K225	L226	E227	L229	Q231	H232	L234	R235	W236	G237	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
V423	E325	S187	LEU	E257	T190	L193	F196	K198	Q199	N200	P201	D202	I203	V204	Y208	M209	D210	V214	G215	S216	D217	L218	E219	I220	G221	Q222	H223	R224	K226	L227	E228	L230	Q232	H233	L235	R236	W237	G238	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
E424	E326	S188	TRP	E258	T191	L194	F197	K199	Q200	N201	P202	D203	I204	V205	Y209	M210	D211	V215	G216	S217	D218	L219	E220	I221	G222	Q223	H224	R225	K227	L228	E229	L231	Q233	H234	L236	R237	W238	G239	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
L425	E327	S189	LEU	E259	T192	L195	F198	K200	Q201	N202	P203	D204	I205	V206	Y210	M211	D212	V216	G217	S218	D219	L220	E221	I222	G223	Q224	H225	R226	K228	L229	E230	L232	Q234	H235	L237	R238	W239	G240	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
W426	E328	S190	TRP	E260	T193	L196	F199	K201	Q202	N203	P204	D205	I206	V207	Y211	M212	D213	V217	G218	S219	D220	L221	E222	I223	G224	Q225	H226	R227	K229	L230	E231	L233	Q235	H236	L238	R239	W240	G241	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
L427	E329	S191	LEU	E261	T194	L197	F200	K202	Q203	N204	P205	D206	I207	V208	Y212	M213	D214	V218	G219	S220	D221	L222	E223	I224	G225	Q226	H227	R228	K230	L231	E232	L234	Q236	H237	L239	R240	W241	G242	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU				
Q428	E330	S192	TRP	E262	T195	L198	F201	K203	Q204	N205	P206	D207																																									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.10Å 115.00Å 65.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-2.80) 94.9 (30.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 2.76Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.295 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7687	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: CSD, FPT

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	0.52	0/4416	1.01	17/6002 (0.3%)
2	B	0.52	0/3420	1.02	19/4646 (0.4%)
All	All	0.52	0/7836	1.01	36/10648 (0.3%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	LEU	N-CA-C	-10.97	100.02	113.41
2	B	132	ILE	N-CA-C	-9.74	97.92	107.76
2	B	420	PRO	CA-C-N	7.94	129.77	119.84
2	B	420	PRO	C-N-CA	7.94	129.77	119.84
1	A	343	GLN	N-CA-C	-7.81	103.71	113.55
2	B	235	HIS	CA-C-N	7.63	127.17	119.24
2	B	235	HIS	C-N-CA	7.63	127.17	119.24
2	B	343	GLN	N-CA-C	-7.62	104.59	114.04
2	B	386	THR	N-CA-C	-7.60	100.49	110.07
1	A	234	LEU	N-CA-C	7.42	120.75	108.96
1	A	142	ILE	N-CA-C	7.21	120.02	109.63
1	A	92	LEU	N-CA-C	-7.17	104.52	113.55
1	A	39	THR	N-CA-C	-6.51	104.03	112.68
2	B	139	THR	CA-C-N	6.26	127.67	119.84
2	B	139	THR	C-N-CA	6.26	127.67	119.84
1	A	442	VAL	N-CA-C	6.16	117.45	108.58
1	A	192	ASP	N-CA-C	-5.94	105.95	112.72
2	B	165	THR	N-CA-C	-5.82	105.01	111.36
1	A	316	GLY	N-CA-C	-5.52	100.69	111.12
1	A	299	ALA	N-CA-C	-5.48	105.22	111.14
1	A	141	GLY	N-CA-C	-5.48	100.20	113.18
1	A	529	GLU	N-CA-C	-5.46	106.29	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	ILE	N-CA-C	5.42	115.67	110.74
2	B	365	VAL	N-CA-C	5.42	115.56	110.30
1	A	204	GLU	N-CA-C	-5.32	105.39	111.14
2	B	131	THR	CA-C-N	-5.30	118.77	122.59
2	B	131	THR	C-N-CA	-5.30	118.77	122.59
1	A	129	ALA	N-CA-C	5.29	117.91	110.23
1	A	325	LEU	N-CA-C	-5.29	101.65	110.17
2	B	312	GLU	N-CA-C	5.26	114.36	108.25
2	B	147	ASN	N-CA-C	-5.23	107.45	113.88
1	A	250	ASP	N-CA-C	-5.23	107.03	113.41
2	B	177	ASP	N-CA-C	-5.17	106.75	113.16
1	A	508	ALA	N-CA-C	-5.14	106.52	112.89
2	B	282	LEU	N-CA-C	-5.08	106.59	112.89
2	B	206	ARG	N-CA-C	-5.08	105.64	111.07

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	4310	0	4342	285	0
2	B	3327	0	3355	189	0
3	A	24	0	16	1	0
4	A	18	0	0	3	0
4	B	8	0	0	2	0
All	All	7687	0	7713	465	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 30.

All (465) 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:139:THR:HB	1:A:140:PRO:HD2	1.21	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.36	1.04
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.06	1.02
1:A:139:THR:HB	1:A:140:PRO:CD	1.99	0.93
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.55	0.87
2:B:393:ILE:HG12	2:B:394:GLN:H	1.40	0.86
2:B:94:ILE:HB	2:B:95:PRO:HA	1.55	0.86
1:A:57:ASN:HD22	1:A:143:ARG:HH12	1.25	0.85
1:A:237:ASP:HB2	1:A:238:LYS:HD3	1.58	0.84
1:A:57:ASN:HD22	1:A:143:ARG:NH1	1.74	0.83
2:B:270:ILE:O	2:B:272:PRO:HD3	1.78	0.82
1:A:400:THR:HG22	1:A:404:GLU:OE2	1.79	0.82
2:B:103:LYS:NZ	2:B:103:LYS:HB2	1.95	0.82
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.77	0.82
1:A:65:LYS:HB3	1:A:68:SER:HB3	1.62	0.81
2:B:161:GLN:HE21	2:B:161:GLN:HA	1.44	0.81
1:A:224:GLU:HB2	1:A:225:PRO:HD2	1.61	0.80
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.63	0.80
1:A:280:CSD:C	1:A:281:LYS:N	2.45	0.80
1:A:395:LYS:HD3	1:A:395:LYS:H	1.48	0.79
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.20	0.77
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.65	0.77
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.66	0.77
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.66	0.77
2:B:266:TRP:O	2:B:269:GLN:HG2	1.86	0.76
1:A:337:TRP:NE1	1:A:367:GLN:HE21	1.82	0.75
1:A:27:THR:HG22	1:A:29:GLU:H	1.52	0.74
2:B:388:LYS:HD3	2:B:388:LYS:C	2.12	0.74
2:B:22:LYS:HA	4:B:1016:HOH:O	1.88	0.74
2:B:163:SER:O	2:B:167:ILE:HG22	1.87	0.73
1:A:33:ALA:O	1:A:37:ILE:HG12	1.89	0.72
2:B:326:ILE:N	2:B:326:ILE:HD12	2.04	0.72
1:A:368:LEU:O	1:A:372:VAL:HG23	1.90	0.72
1:A:197:GLN:O	1:A:200:THR:HB	1.91	0.71
2:B:142:ILE:N	2:B:142:ILE:HD12	2.04	0.71
2:B:16:MET:HE3	2:B:83:ARG:HA	1.71	0.71
2:B:107:THR:O	2:B:189:VAL:HG22	1.91	0.71
2:B:31:ILE:O	2:B:35:VAL:HG23	1.90	0.71
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.26	0.71
1:A:195:ILE:HD13	1:A:195:ILE:N	2.05	0.71
2:B:189:VAL:HG21	2:B:202:ILE:HD12	1.74	0.70
1:A:220:LYS:NZ	1:A:220:LYS:HB3	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HD13	1:A:302:GLU:OE1	1.91	0.70
2:B:393:ILE:HG12	2:B:394:GLN:N	2.06	0.70
1:A:57:ASN:HA	1:A:129:ALA:O	1.91	0.70
2:B:242:GLN:HE21	2:B:353:LYS:HD3	1.55	0.70
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.27	0.70
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.73	0.69
1:A:11:LYS:O	1:A:85:GLN:HG2	1.93	0.69
1:A:65:LYS:HE2	1:A:65:LYS:HA	1.72	0.69
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.28	0.69
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.17	0.69
2:B:94:ILE:HB	2:B:95:PRO:CA	2.23	0.69
2:B:142:ILE:HD12	2:B:142:ILE:H	1.56	0.68
1:A:167:ILE:O	1:A:170:PRO:HD2	1.93	0.68
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.76	0.68
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.24	0.68
1:A:253:THR:HG23	1:A:255:ASN:H	1.59	0.68
2:B:89:GLU:C	2:B:93:GLY:HA3	2.19	0.68
2:B:319:TYR:OH	2:B:385:LYS:HE2	1.93	0.68
1:A:164:MET:HG3	1:A:168:LEU:HD22	1.74	0.68
2:B:103:LYS:HB2	2:B:103:LYS:HZ3	1.58	0.67
1:A:56:TYR:O	1:A:143:ARG:NH2	2.27	0.67
2:B:79:GLU:HG3	2:B:83:ARG:HD3	1.75	0.67
1:A:418:ASN:C	1:A:418:ASN:HD22	2.02	0.67
1:A:428:GLN:HA	1:A:509:GLN:NE2	2.11	0.66
2:B:166:LYS:HB2	2:B:166:LYS:HZ2	1.61	0.66
2:B:278:GLN:HB3	2:B:299:ALA:HA	1.76	0.66
1:A:264:LEU:HD23	1:A:276:VAL:HG12	1.77	0.66
1:A:27:THR:HB	1:A:30:LYS:HG3	1.76	0.66
1:A:110:ASP:O	1:A:217:PRO:HD3	1.95	0.66
2:B:371:ALA:O	2:B:375:ILE:HG13	1.95	0.66
1:A:195:ILE:HD13	1:A:195:ILE:H	1.59	0.66
1:A:395:LYS:H	1:A:395:LYS:CD	2.08	0.65
2:B:27:THR:OG1	2:B:30:LYS:HD3	1.96	0.65
2:B:103:LYS:HG2	2:B:191:SER:N	2.10	0.65
2:B:422:LEU:O	2:B:425:LEU:HB3	1.97	0.65
1:A:26:LEU:HB2	1:A:31:ILE:HD11	1.79	0.64
1:A:70:LYS:HG2	1:A:71:TRP:H	1.61	0.64
2:B:393:ILE:CG1	2:B:394:GLN:H	2.10	0.64
1:A:126:LYS:HE2	1:A:127:TYR:CZ	2.33	0.64
1:A:296:THR:HG22	1:A:297:GLU:N	2.12	0.64
1:A:484:LEU:O	1:A:487:GLN:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:C	2:B:170:PRO:HD2	2.23	0.63
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.80	0.63
2:B:277:ARG:O	2:B:281:LYS:HG3	1.98	0.63
1:A:46:LYS:HD3	1:A:116:PHE:CD2	2.34	0.63
1:A:281:LYS:HD2	1:A:284:ARG:NH1	2.14	0.63
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.63
1:A:337:TRP:CZ3	1:A:368:LEU:HD23	2.34	0.63
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.13	0.62
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.81	0.62
1:A:195:ILE:HG12	1:A:196:GLY:H	1.65	0.62
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.15	0.62
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.35	0.61
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.65	0.61
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.34	0.61
2:B:104:LYS:O	2:B:236:PRO:HD2	1.99	0.61
1:A:201:LYS:HD3	1:A:204:GLU:CD	2.25	0.61
1:A:62:ALA:C	1:A:63:ILE:HD12	2.25	0.61
2:B:103:LYS:HG2	2:B:191:SER:CA	2.30	0.61
2:B:169:GLU:N	2:B:170:PRO:HD2	2.15	0.61
1:A:391:LEU:C	1:A:417:VAL:HG12	2.25	0.60
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.82	0.60
2:B:365:VAL:O	2:B:369:THR:HG23	2.01	0.60
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.84	0.59
2:B:174:GLN:C	2:B:176:PRO:HD3	2.27	0.59
1:A:57:ASN:ND2	1:A:143:ARG:HH12	1.99	0.59
1:A:516:GLU:N	1:A:516:GLU:OE1	2.35	0.59
2:B:160:PHE:HD1	2:B:164:MET:HB2	1.67	0.59
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.83	0.59
1:A:225:PRO:HA	1:A:226:PRO:C	2.28	0.59
1:A:279:LEU:O	1:A:282:LEU:HB2	2.03	0.59
2:B:350:LYS:HE2	2:B:378:GLU:OE1	2.03	0.59
1:A:46:LYS:HD3	1:A:116:PHE:HD2	1.66	0.59
1:A:340:GLN:HA	1:A:351:THR:HA	1.85	0.59
1:A:57:ASN:HB2	1:A:143:ARG:HH12	1.67	0.59
1:A:136:ASN:HB3	1:A:139:THR:HG21	1.85	0.58
1:A:368:LEU:HD13	1:A:368:LEU:C	2.28	0.58
1:A:469:LEU:HD23	1:A:469:LEU:N	2.19	0.58
1:A:332:GLN:HB2	1:A:338:THR:HG23	1.85	0.58
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.84	0.58
2:B:205:LEU:O	2:B:209:LEU:HG	2.04	0.58
1:A:5:ILE:HD12	1:A:5:ILE:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:O	1:A:200:THR:N	2.36	0.58
1:A:104:LYS:HZ3	1:A:104:LYS:HB2	1.69	0.57
1:A:114:ALA:O	1:A:118:VAL:HG23	2.03	0.57
2:B:205:LEU:HD22	2:B:209:LEU:HG	1.85	0.57
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.85	0.57
1:A:348:ASN:ND2	1:A:351:THR:HG22	2.19	0.57
1:A:455:ALA:O	1:A:467:VAL:HG22	2.05	0.57
1:A:56:TYR:O	1:A:57:ASN:HB2	2.04	0.57
1:A:395:LYS:HD3	1:A:395:LYS:N	2.19	0.57
2:B:116:PHE:HD1	2:B:148:VAL:HG21	1.69	0.57
2:B:369:THR:O	2:B:373:GLN:HG3	2.04	0.57
1:A:37:ILE:O	1:A:41:MET:HG3	2.05	0.56
1:A:5:ILE:HD12	1:A:5:ILE:N	2.20	0.56
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.88	0.56
1:A:126:LYS:HE2	1:A:127:TYR:CE2	2.40	0.56
2:B:401:TRP:O	2:B:404:GLU:HB2	2.05	0.56
1:A:31:ILE:HD12	1:A:133:PRO:HB2	1.87	0.56
1:A:335:GLY:O	1:A:355:ALA:HA	2.06	0.56
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.40	0.56
2:B:207:GLN:O	2:B:211:ARG:HG2	2.05	0.56
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.87	0.56
1:A:253:THR:HG22	1:A:256:ASP:CG	2.30	0.55
2:B:89:GLU:O	2:B:93:GLY:HA3	2.07	0.55
2:B:278:GLN:HB3	2:B:299:ALA:CA	2.37	0.55
2:B:366:LYS:O	2:B:370:GLU:HG3	2.07	0.55
2:B:103:LYS:HG3	2:B:192:ASP:OD1	2.06	0.55
2:B:118:VAL:HB	2:B:149:LEU:HG	1.89	0.55
1:A:31:ILE:CD1	1:A:133:PRO:HB2	2.37	0.55
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.89	0.55
2:B:193:LEU:HD23	2:B:197:GLN:HG2	1.88	0.54
2:B:420:PRO:HG2	2:B:423:VAL:CG2	2.37	0.54
1:A:26:LEU:HD12	1:A:133:PRO:HD2	1.89	0.54
1:A:151:GLN:CD	1:A:151:GLN:H	2.13	0.54
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.88	0.54
2:B:172:ARG:O	2:B:176:PRO:HG3	2.07	0.54
2:B:201:LYS:HZ3	2:B:204:GLU:CD	2.14	0.54
2:B:420:PRO:HG2	2:B:423:VAL:HG23	1.90	0.54
1:A:63:ILE:HD12	1:A:63:ILE:N	2.22	0.54
1:A:401:TRP:HA	1:A:404:GLU:OE2	2.07	0.54
2:B:164:MET:O	2:B:167:ILE:HG23	2.08	0.54
2:B:171:PHE:HD1	2:B:208:HIS:ND1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PHE:CD2	2:B:403:THR:HG21	2.42	0.54
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.90	0.54
1:A:115:TYR:O	1:A:149:LEU:HB2	2.07	0.54
1:A:170:PRO:O	1:A:173:LYS:HB3	2.08	0.54
1:A:296:THR:HG22	1:A:297:GLU:H	1.73	0.54
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.71	0.54
1:A:247:PRO:O	1:A:307:ARG:NH2	2.41	0.54
2:B:326:ILE:HD12	2:B:326:ILE:H	1.71	0.54
1:A:260:LEU:HD22	1:A:264:LEU:HD13	1.89	0.53
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.06	0.53
1:A:17:ASP:O	1:A:83:ARG:NE	2.41	0.53
1:A:516:GLU:HG2	1:A:517:LEU:N	2.22	0.53
2:B:151:GLN:CD	2:B:151:GLN:H	2.16	0.53
1:A:253:THR:HG22	1:A:256:ASP:H	1.72	0.53
1:A:328:GLU:O	1:A:339:TYR:HA	2.08	0.53
1:A:63:ILE:HG22	1:A:64:LYS:N	2.22	0.53
2:B:423:VAL:HA	2:B:426:TRP:CE3	2.43	0.53
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.24	0.53
2:B:189:VAL:HG23	2:B:189:VAL:O	2.09	0.53
1:A:209:LEU:O	1:A:214:LEU:HB2	2.09	0.53
1:A:170:PRO:O	1:A:171:PHE:C	2.51	0.53
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.44	0.52
2:B:174:GLN:C	2:B:174:GLN:HE21	2.16	0.52
1:A:312:GLU:O	1:A:312:GLU:HG2	2.09	0.52
1:A:348:ASN:ND2	1:A:351:THR:CG2	2.71	0.52
2:B:163:SER:O	2:B:166:LYS:HB3	2.07	0.52
1:A:260:LEU:HD13	1:A:264:LEU:HD22	1.92	0.52
1:A:424:LYS:NZ	1:A:426:TRP:CE3	2.76	0.52
2:B:284:ARG:O	2:B:287:LYS:NZ	2.42	0.52
2:B:328:GLU:O	2:B:339:TYR:HA	2.08	0.52
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.24	0.52
1:A:208:HIS:HA	1:A:211:ARG:HG3	1.92	0.52
1:A:503:LEU:O	1:A:507:GLN:HG3	2.10	0.52
1:A:518:VAL:O	1:A:522:ILE:HG13	2.10	0.52
1:A:280:CSD:O	1:A:281:LYS:HA	2.10	0.52
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.45	0.52
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.45	0.52
1:A:500:GLN:CD	1:A:500:GLN:H	2.18	0.52
2:B:60:VAL:HG21	2:B:73:LYS:HZ1	1.75	0.51
1:A:78:ARG:O	1:A:82:LYS:HG3	2.10	0.51
1:A:280:CSD:C	1:A:281:LYS:CA	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ILE:H	2:B:142:ILE:CD1	2.23	0.51
1:A:374:LYS:HD3	1:A:374:LYS:C	2.36	0.51
1:A:492:GLU:CD	1:A:530:LYS:HE2	2.35	0.51
1:A:31:ILE:HG23	1:A:133:PRO:O	2.11	0.51
1:A:142:ILE:HD12	1:A:144:TYR:OH	2.10	0.51
2:B:388:LYS:CE	2:B:415:GLU:HB2	2.40	0.51
1:A:40:GLU:HG3	1:A:44:GLU:OE1	2.11	0.51
1:A:368:LEU:O	1:A:368:LEU:HD13	2.10	0.51
2:B:100:LEU:HB2	2:B:179:VAL:HG11	1.92	0.51
1:A:57:ASN:ND2	1:A:143:ARG:NH1	2.53	0.51
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.44	0.51
2:B:326:ILE:HG22	2:B:327:ALA:N	2.26	0.51
2:B:314:VAL:O	2:B:317:VAL:HG22	2.11	0.50
1:A:337:TRP:NE1	1:A:367:GLN:HG2	2.27	0.50
2:B:9:PRO:HB2	4:B:1014:HOH:O	2.11	0.50
1:A:5:ILE:HG21	1:A:163:SER:HB3	1.93	0.50
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.94	0.50
1:A:503:LEU:HD13	1:A:507:GLN:HG3	1.94	0.50
1:A:125:ARG:HB3	1:A:145:GLN:NE2	2.27	0.50
1:A:198:HIS:C	1:A:200:THR:N	2.69	0.50
1:A:134:SER:HB3	1:A:141:GLY:N	2.27	0.50
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.11	0.50
2:B:208:HIS:HA	2:B:211:ARG:HG3	1.93	0.50
2:B:234:LEU:HD11	2:B:377:THR:CG2	2.42	0.50
1:A:28:GLU:O	1:A:32:LYS:HG3	2.11	0.50
1:A:344:GLU:O	1:A:347:LYS:HB2	2.12	0.50
1:A:399:GLU:O	1:A:402:TRP:HB3	2.12	0.50
2:B:49:LYS:HA	2:B:143:ARG:O	2.11	0.50
1:A:400:THR:O	1:A:404:GLU:HG3	2.12	0.49
1:A:317:VAL:HG22	1:A:318:TYR:H	1.76	0.49
2:B:142:ILE:N	2:B:142:ILE:CD1	2.74	0.49
1:A:412:PRO:HG3	2:B:401:TRP:CH2	2.48	0.49
1:A:406:TRP:O	2:B:331:LYS:HB3	2.12	0.49
1:A:428:GLN:HA	1:A:509:GLN:HE22	1.78	0.49
2:B:89:GLU:CA	2:B:93:GLY:HA3	2.43	0.49
2:B:208:HIS:CD2	2:B:212:TRP:HZ3	2.30	0.49
2:B:263:LYS:HE3	2:B:426:TRP:HA	1.95	0.49
2:B:277:ARG:HG3	2:B:277:ARG:HH11	1.76	0.49
1:A:260:LEU:CD1	1:A:264:LEU:HD22	2.42	0.49
1:A:108:VAL:C	1:A:109:LEU:HD12	2.38	0.49
1:A:70:LYS:HG2	1:A:71:TRP:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.47	0.49
2:B:278:GLN:HB3	2:B:299:ALA:CB	2.43	0.49
1:A:164:MET:CG	1:A:182:GLN:HE21	2.25	0.48
1:A:198:HIS:C	1:A:200:THR:H	2.20	0.48
2:B:189:VAL:HG21	2:B:202:ILE:CD1	2.42	0.48
2:B:388:LYS:C	2:B:388:LYS:CD	2.86	0.48
1:A:40:GLU:HG2	4:A:1022:HOH:O	2.13	0.48
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.48	0.48
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.48	0.48
1:A:307:ARG:O	1:A:311:LYS:HG3	2.14	0.48
2:B:162:SER:OG	2:B:163:SER:N	2.47	0.48
1:A:126:LYS:HA	1:A:145:GLN:OE1	2.14	0.48
1:A:134:SER:HB3	1:A:140:PRO:HG2	1.95	0.48
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.95	0.48
2:B:388:LYS:HE2	2:B:415:GLU:HB2	1.96	0.48
1:A:131:THR:OG1	1:A:143:ARG:HG2	2.14	0.48
1:A:499:SER:HA	4:A:1013:HOH:O	2.13	0.48
2:B:326:ILE:N	2:B:326:ILE:CD1	2.75	0.47
1:A:220:LYS:HB3	1:A:220:LYS:HZ3	1.75	0.47
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.48	0.47
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.49	0.47
1:A:337:TRP:HE1	1:A:367:GLN:HG2	1.78	0.47
1:A:429:LEU:H	1:A:509:GLN:HE21	1.62	0.47
2:B:175:ASN:ND2	2:B:201:LYS:CE	2.78	0.47
2:B:107:THR:HB	2:B:189:VAL:CG2	2.44	0.47
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.48	0.47
2:B:169:GLU:OE1	2:B:170:PRO:HD3	2.15	0.47
2:B:278:GLN:CB	2:B:299:ALA:HA	2.42	0.47
1:A:51:GLY:C	1:A:53:GLU:H	2.21	0.47
1:A:229:TRP:O	1:A:230:MET:C	2.58	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.47
2:B:76:ASP:OD2	2:B:78:ARG:HB2	2.15	0.47
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.15	0.47
1:A:129:ALA:HB1	1:A:143:ARG:NH2	2.30	0.47
1:A:429:LEU:H	1:A:509:GLN:NE2	2.12	0.47
2:B:13:LYS:HD2	2:B:16:MET:HE2	1.95	0.47
1:A:254:VAL:HG23	1:A:291:GLU:O	2.14	0.47
1:A:224:GLU:HA	1:A:227:PHE:CZ	2.50	0.47
2:B:83:ARG:H	2:B:83:ARG:HG2	1.55	0.47
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.15	0.47
1:A:28:GLU:OE2	1:A:135:ILE:HG12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:HG2	1:A:56:TYR:H	1.81	0.46
1:A:109:LEU:O	1:A:186:ASP:HA	2.15	0.46
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.80	0.46
1:A:458:VAL:HG23	1:A:458:VAL:O	2.14	0.46
1:A:108:VAL:HA	1:A:187:LEU:O	2.15	0.46
1:A:151:GLN:H	1:A:151:GLN:NE2	2.12	0.46
1:A:164:MET:HE3	1:A:187:LEU:HD11	1.98	0.46
1:A:194:GLU:O	1:A:195:ILE:C	2.58	0.46
1:A:225:PRO:HD3	1:A:227:PHE:CE2	2.51	0.46
1:A:511:ASP:OD1	1:A:512:GLN:HG2	2.15	0.46
2:B:253:THR:O	2:B:257:ILE:HG12	2.16	0.46
1:A:27:THR:HG22	1:A:29:GLU:HB3	1.97	0.46
1:A:280:CSD:C	1:A:281:LYS:HA	2.44	0.46
1:A:291:GLU:HG2	1:A:293:ILE:HD12	1.96	0.46
1:A:332:GLN:O	1:A:332:GLN:HG2	2.16	0.46
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.37	0.46
1:A:522:ILE:O	1:A:526:ILE:HG13	2.15	0.46
2:B:102:LYS:O	2:B:104:LYS:N	2.43	0.46
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.51	0.46
1:A:234:LEU:HD12	3:A:999:FPT:HB1	1.97	0.46
2:B:160:PHE:CD1	2:B:164:MET:HB2	2.50	0.46
2:B:254:VAL:HG23	2:B:291:GLU:O	2.16	0.46
1:A:136:ASN:HB3	1:A:139:THR:CG2	2.44	0.46
2:B:104:LYS:CB	2:B:192:ASP:HA	2.46	0.46
2:B:296:THR:O	2:B:297:GLU:C	2.59	0.46
1:A:270:ILE:O	1:A:272:PRO:HD3	2.16	0.46
1:A:516:GLU:O	1:A:517:LEU:C	2.58	0.46
1:A:477:THR:O	1:A:480:GLN:HB3	2.15	0.46
2:B:428:GLN:C	2:B:428:GLN:NE2	2.74	0.46
1:A:101:LYS:HG2	1:A:321:PRO:HD3	1.97	0.46
1:A:344:GLU:O	1:A:347:LYS:N	2.35	0.46
2:B:106:VAL:HG13	2:B:189:VAL:C	2.41	0.46
2:B:160:PHE:O	2:B:161:GLN:C	2.59	0.46
2:B:175:ASN:C	2:B:177:ASP:H	2.24	0.46
2:B:183:TYR:OH	2:B:386:THR:HG23	2.16	0.46
1:A:469:LEU:HD23	1:A:469:LEU:H	1.81	0.45
2:B:81:ASN:OD1	2:B:153:TRP:HA	2.16	0.45
1:A:500:GLN:N	1:A:500:GLN:OE1	2.49	0.45
2:B:100:LEU:O	2:B:102:LYS:N	2.49	0.45
1:A:369:THR:O	1:A:372:VAL:HB	2.16	0.45
1:A:494:ASN:OD1	1:A:532:TYR:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:PRO:C	2:B:16:MET:H	2.25	0.45
2:B:339:TYR:C	2:B:340:GLN:NE2	2.75	0.45
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.98	0.45
1:A:107:THR:OG1	1:A:202:ILE:HD12	2.17	0.45
2:B:166:LYS:O	2:B:169:GLU:HG3	2.16	0.45
1:A:54:ASN:ND2	1:A:126:LYS:HB2	2.31	0.45
1:A:88:TRP:O	1:A:89:GLU:HB2	2.17	0.45
2:B:111:VAL:O	2:B:112:GLY:C	2.60	0.45
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.40	0.45
1:A:249:LYS:HZ1	1:A:256:ASP:CG	2.25	0.45
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.52	0.45
2:B:406:TRP:HZ2	2:B:410:TRP:O	1.99	0.45
1:A:201:LYS:HA	1:A:204:GLU:HG3	1.99	0.44
1:A:257:ILE:O	1:A:261:VAL:HG23	2.17	0.44
1:A:292:VAL:C	1:A:293:ILE:HD12	2.42	0.44
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.52	0.44
1:A:65:LYS:HB3	1:A:68:SER:CB	2.41	0.44
2:B:12:LEU:HD12	2:B:124:PHE:CE1	2.52	0.44
1:A:182:GLN:HB3	4:A:1026:HOH:O	2.17	0.44
1:A:291:GLU:HG2	1:A:293:ILE:CD1	2.47	0.44
1:A:30:LYS:O	1:A:31:ILE:C	2.60	0.44
1:A:64:LYS:HG2	1:A:70:LYS:O	2.18	0.44
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.52	0.44
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.18	0.44
2:B:100:LEU:C	2:B:102:LYS:H	2.25	0.44
2:B:168:LEU:O	2:B:172:ARG:HG3	2.17	0.44
2:B:282:LEU:HD22	2:B:293:ILE:CG2	2.48	0.44
2:B:296:THR:O	2:B:299:ALA:N	2.51	0.44
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.52	0.44
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.99	0.44
1:A:296:THR:CG2	1:A:297:GLU:N	2.80	0.44
2:B:166:LYS:HZ2	2:B:166:LYS:CB	2.27	0.44
2:B:255:ASN:O	2:B:258:GLN:HB2	2.18	0.44
1:A:406:TRP:CE3	1:A:407:GLN:N	2.86	0.43
1:A:65:LYS:HE2	1:A:65:LYS:CA	2.45	0.43
1:A:457:TYR:CD1	1:A:457:TYR:C	2.96	0.43
2:B:38:CYS:SG	2:B:73:LYS:NZ	2.76	0.43
1:A:160:PHE:HE1	1:A:184:MET:O	2.01	0.43
1:A:174:GLN:HE21	1:A:174:GLN:HB2	1.52	0.43
1:A:505:ILE:O	1:A:508:ALA:HB3	2.18	0.43
2:B:103:LYS:O	2:B:191:SER:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:NZ	1:A:256:ASP:CG	2.77	0.43
1:A:283:LEU:C	1:A:286:THR:HG23	2.44	0.43
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.83	0.43
1:A:22:LYS:NZ	1:A:24:TRP:HA	2.34	0.43
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.84	0.43
1:A:469:LEU:N	1:A:469:LEU:CD2	2.82	0.43
2:B:87:PHE:O	2:B:89:GLU:N	2.52	0.43
1:A:7:THR:HG21	1:A:121:ASP:HA	2.00	0.43
1:A:248:GLU:HG3	1:A:248:GLU:O	2.19	0.43
1:A:257:ILE:O	1:A:258:GLN:C	2.60	0.43
2:B:166:LYS:HZ1	2:B:166:LYS:HA	1.84	0.43
2:B:379:SER:CB	2:B:387:PRO:HD3	2.48	0.43
1:A:283:LEU:O	1:A:286:THR:HG23	2.20	0.42
1:A:246:LEU:HD12	1:A:307:ARG:HG2	2.01	0.42
1:A:280:CSD:O	1:A:281:LYS:CA	2.68	0.42
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.32	0.42
1:A:293:ILE:HD12	1:A:293:ILE:N	2.34	0.42
1:A:486:LEU:HD13	1:A:524:GLN:HB2	2.01	0.42
2:B:103:LYS:NZ	2:B:103:LYS:CB	2.77	0.42
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.34	0.42
1:A:253:THR:HG23	1:A:254:VAL:N	2.35	0.42
1:A:298:GLU:HA	1:A:301:LEU:HB2	2.02	0.42
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.02	0.42
2:B:94:ILE:HG12	2:B:161:GLN:OE1	2.19	0.42
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.73	0.42
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.53	0.42
1:A:232:TYR:CD1	1:A:232:TYR:N	2.87	0.42
1:A:401:TRP:CH2	1:A:409:THR:HG21	2.55	0.42
2:B:120:LEU:O	2:B:121:ASP:C	2.63	0.42
1:A:104:LYS:CB	1:A:192:ASP:HA	2.49	0.42
1:A:195:ILE:N	1:A:195:ILE:CD1	2.74	0.42
1:A:253:THR:HG23	1:A:255:ASN:N	2.31	0.42
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.19	0.42
2:B:278:GLN:HB3	2:B:299:ALA:HB2	2.02	0.42
2:B:394:GLN:O	2:B:395:LYS:C	2.63	0.42
1:A:344:GLU:CB	1:A:347:LYS:HD2	2.50	0.42
1:A:426:TRP:H	1:A:426:TRP:CD1	2.37	0.42
2:B:169:GLU:N	2:B:170:PRO:CD	2.81	0.42
2:B:175:ASN:N	2:B:176:PRO:HD3	2.35	0.42
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.84	0.42
1:A:63:ILE:HG22	1:A:64:LYS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HB2	1:A:249:LYS:HG2	2.01	0.42
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.92	0.42
2:B:257:ILE:O	2:B:260:LEU:HB3	2.19	0.42
2:B:296:THR:O	2:B:298:GLU:N	2.53	0.42
1:A:74:LEU:C	1:A:74:LEU:CD2	2.93	0.41
1:A:138:GLU:O	1:A:139:THR:HG23	2.20	0.41
1:A:279:LEU:N	1:A:279:LEU:CD1	2.83	0.41
2:B:76:ASP:C	2:B:78:ARG:H	2.28	0.41
1:A:417:VAL:O	1:A:419:THR:N	2.52	0.41
1:A:136:ASN:OD1	1:A:139:THR:HG23	2.20	0.41
1:A:356:ARG:HE	1:A:358:ARG:NH1	2.18	0.41
2:B:198:HIS:C	2:B:200:THR:N	2.77	0.41
2:B:263:LYS:HG3	2:B:426:TRP:CD1	2.56	0.41
2:B:305:GLU:O	2:B:306:ASN:C	2.62	0.41
1:A:54:ASN:OD1	1:A:56:TYR:HB2	2.20	0.41
1:A:417:VAL:O	1:A:417:VAL:HG13	2.20	0.41
2:B:241:VAL:O	2:B:243:PRO:HD3	2.20	0.41
1:A:481:ALA:O	1:A:482:ILE:C	2.63	0.41
2:B:161:GLN:O	2:B:162:SER:C	2.64	0.41
1:A:317:VAL:HG22	1:A:318:TYR:N	2.36	0.41
1:A:28:GLU:OE2	1:A:135:ILE:HG23	2.21	0.41
1:A:164:MET:HB3	1:A:182:GLN:HE21	1.85	0.41
1:A:253:THR:HA	1:A:292:VAL:HA	2.02	0.41
2:B:53:GLU:O	2:B:55:PRO:HD3	2.21	0.41
1:A:12:LEU:HD11	1:A:127:TYR:CD1	2.55	0.41
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.50	0.41
1:A:433:PRO:HA	1:A:532:TYR:CG	2.55	0.41
2:B:257:ILE:O	2:B:261:VAL:HG23	2.21	0.41
2:B:379:SER:HA	2:B:383:TRP:CE3	2.56	0.41
1:A:111:VAL:HG23	1:A:111:VAL:O	2.20	0.41
1:A:151:GLN:CD	1:A:151:GLN:N	2.78	0.41
1:A:240:THR:OG1	1:A:241:VAL:N	2.53	0.41
1:A:271:TYR:OH	1:A:313:PRO:HA	2.21	0.41
1:A:436:GLY:O	1:A:461:ARG:NH2	2.53	0.41
1:A:473:THR:H	1:A:476:LYS:HB3	1.85	0.41
1:A:520:GLN:O	1:A:523:GLU:HB3	2.21	0.41
2:B:11:LYS:O	2:B:85:GLN:HG2	2.20	0.41
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.81	0.41
1:A:32:LYS:CG	1:A:135:ILE:HD11	2.51	0.41
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.56	0.41
2:B:161:GLN:O	2:B:164:MET:HB3	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:ALA:O	2:B:302:GLU:N	2.54	0.41
2:B:428:GLN:C	2:B:428:GLN:HE21	2.29	0.41
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.56	0.40
1:A:281:LYS:O	1:A:284:ARG:HG3	2.20	0.40
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.56	0.40
2:B:8:VAL:HG11	2:B:159:ILE:HG12	2.03	0.40
2:B:329:ILE:HG22	2:B:330:GLN:N	2.36	0.40
1:A:363:ASN:OD1	1:A:363:ASN:C	2.64	0.40
1:A:498:ASP:HA	1:A:536:VAL:O	2.20	0.40
2:B:129:ALA:HA	2:B:144:TYR:O	2.20	0.40
1:A:282:LEU:HD21	1:A:295:LEU:HD22	2.02	0.40
1:A:473:THR:HB	1:A:476:LYS:HB2	2.02	0.40
2:B:142:ILE:CG2	2:B:144:TYR:CE2	3.04	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	519/560 (93%)	451 (87%)	47 (9%)	21 (4%)	2	8
2	B	396/440 (90%)	342 (86%)	41 (10%)	13 (3%)	3	11
All	All	915/1000 (92%)	793 (87%)	88 (10%)	34 (4%)	2	9

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	140	PRO
1	A	195	ILE
1	A	402	TRP
1	A	412	PRO

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Mol	Chain	Res	Type
1	A	538	ALA
2	B	94	ILE
2	B	95	PRO
1	A	199	ARG
1	A	345	PRO
2	B	101	LYS
2	B	297	GLU
1	A	222	GLN
1	A	230	MET
1	A	528	LYS
2	B	85	GLN
2	B	88	TRP
2	B	103	LYS
2	B	136	ASN
2	B	162	SER
2	B	193	LEU
2	B	233	GLU
1	A	56	TYR
1	A	57	ASN
1	A	139	THR
1	A	198	HIS
1	A	243	PRO
1	A	487	GLN
1	A	170	PRO
1	A	85	GLN
1	A	135	ILE
1	A	268	SER
2	B	195	ILE
2	B	421	PRO

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	473/499 (95%)	430 (91%)	43 (9%)	9	28
2	B	366/400 (92%)	337 (92%)	29 (8%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	839/899 (93%)	767 (91%)	72 (9%)	10	31

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	39	THR
1	A	65	LYS
1	A	74	LEU
1	A	89	GLU
1	A	101	LYS
1	A	104	LYS
1	A	105	SER
1	A	151	GLN
1	A	168	LEU
1	A	174	GLN
1	A	177	ASP
1	A	194	GLU
1	A	195	ILE
1	A	216	THR
1	A	220	LYS
1	A	232	TYR
1	A	238	LYS
1	A	243	PRO
1	A	249	LYS
1	A	253	THR
1	A	259	LYS
1	A	264	LEU
1	A	279	LEU
1	A	282	LEU
1	A	283	LEU
1	A	284	ARG
1	A	289	LEU
1	A	301	LEU
1	A	303	LEU
1	A	340	GLN
1	A	345	PRO
1	A	362	THR
1	A	418	ASN
1	A	463	ARG
1	A	469	LEU

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Mol	Chain	Res	Type
1	A	488	ASP
1	A	493	VAL
1	A	500	GLN
1	A	512	GLN
1	A	517	LEU
1	A	527	LYS
2	B	6	GLU
2	B	8	VAL
2	B	10	VAL
2	B	55	PRO
2	B	83	ARG
2	B	103	LYS
2	B	132	ILE
2	B	142	ILE
2	B	161	GLN
2	B	166	LYS
2	B	167	ILE
2	B	169	GLU
2	B	174	GLN
2	B	205	LEU
2	B	283	LEU
2	B	289	LEU
2	B	290	THR
2	B	298	GLU
2	B	300	GLU
2	B	303	LEU
2	B	314	VAL
2	B	317	VAL
2	B	326	ILE
2	B	368	LEU
2	B	377	THR
2	B	388	LYS
2	B	405	TYR
2	B	410	TRP
2	B	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	147	ASN
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	174	GLN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	221	HIS
1	A	222	GLN
1	A	278	GLN
1	A	332	GLN
1	A	348	ASN
1	A	367	GLN
1	A	418	ASN
1	A	475	GLN
1	A	509	GLN
1	A	512	GLN
1	A	520	GLN
2	B	57	ASN
2	B	91	GLN
2	B	151	GLN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	197	GLN
2	B	235	HIS
2	B	242	GLN
2	B	255	ASN
2	B	269	GLN
2	B	336	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	280	1	4,7,8	1.14	0	1,8,10	6.00	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	280	CSD	OD1-SG-CB	6.00	116.65	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FPT	A	999	-	25,25,25	1.62	6 (24%)	30,32,32	1.96	9 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FPT	A	999	-	-	9/15/15/15	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FPT	C13-N14	3.22	1.38	1.34
3	A	999	FPT	C17-C18	2.94	1.42	1.39
3	A	999	FPT	C1-N2	2.80	1.39	1.34
3	A	999	FPT	C18-C13	2.62	1.42	1.38
3	A	999	FPT	C1-N8	-2.29	1.35	1.40
3	A	999	FPT	C9-N8	-2.09	1.31	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FPT	C15-N14-C13	4.04	122.91	117.79
3	A	999	FPT	C3-N2-C1	3.98	121.56	117.83
3	A	999	FPT	C16-C15-N14	-3.78	119.34	123.97
3	A	999	FPT	C4-C3-N2	-3.27	118.83	123.50
3	A	999	FPT	O17-C17-C18	3.11	120.61	115.92
3	A	999	FPT	O17-C17-C16	-2.79	117.85	123.95
3	A	999	FPT	N8-C1-N2	2.60	122.67	114.87
3	A	999	FPT	C6-C1-N8	-2.30	116.22	123.02
3	A	999	FPT	C16-C17-C18	2.09	121.29	117.88

There are no chirality outliers.

All (9) torsion outliers are listed below:

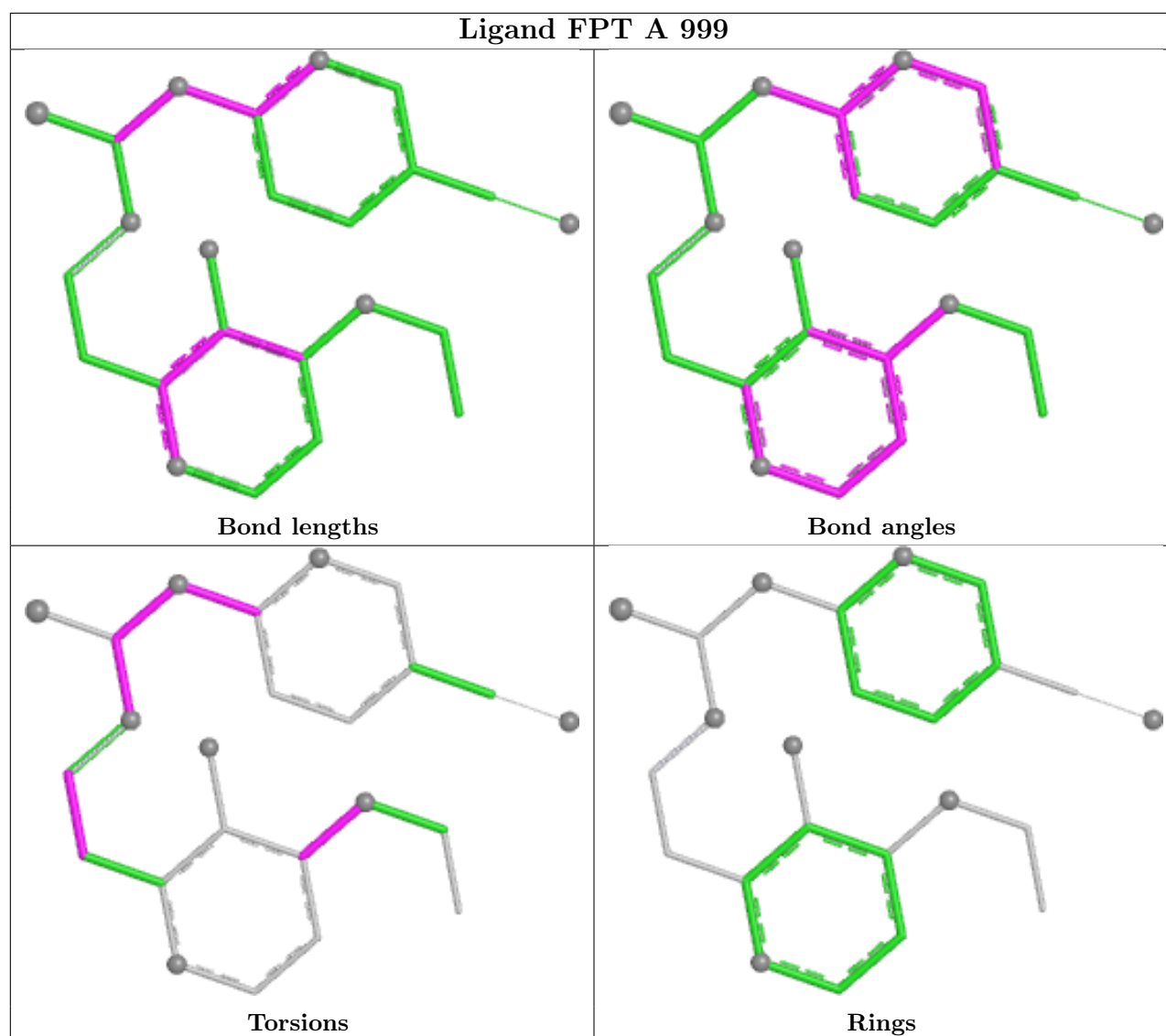
Mol	Chain	Res	Type	Atoms
3	A	999	FPT	N2-C1-N8-C9
3	A	999	FPT	C6-C1-N8-C9
3	A	999	FPT	S9-C9-N8-C1
3	A	999	FPT	N10-C9-N8-C1
3	A	999	FPT	N8-C9-N10-C11
3	A	999	FPT	S9-C9-N10-C11
3	A	999	FPT	N10-C11-C12-C13
3	A	999	FPT	C18-C17-O17-CA
3	A	999	FPT	C16-C17-O17-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	FPT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	280:CSD	C	281:LYS	N	2.45

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	524/560 (93%)	-0.17	0 100 100	23, 62, 104, 140	0
2	B	402/440 (91%)	-0.30	3 (0%) 84 77	26, 57, 103, 144	0
All	All	926/1000 (92%)	-0.23	3 (0%) 90 86	23, 59, 104, 144	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	2.5
2	B	92	LEU	2.2
2	B	90	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.92	0.09	39,49,63,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

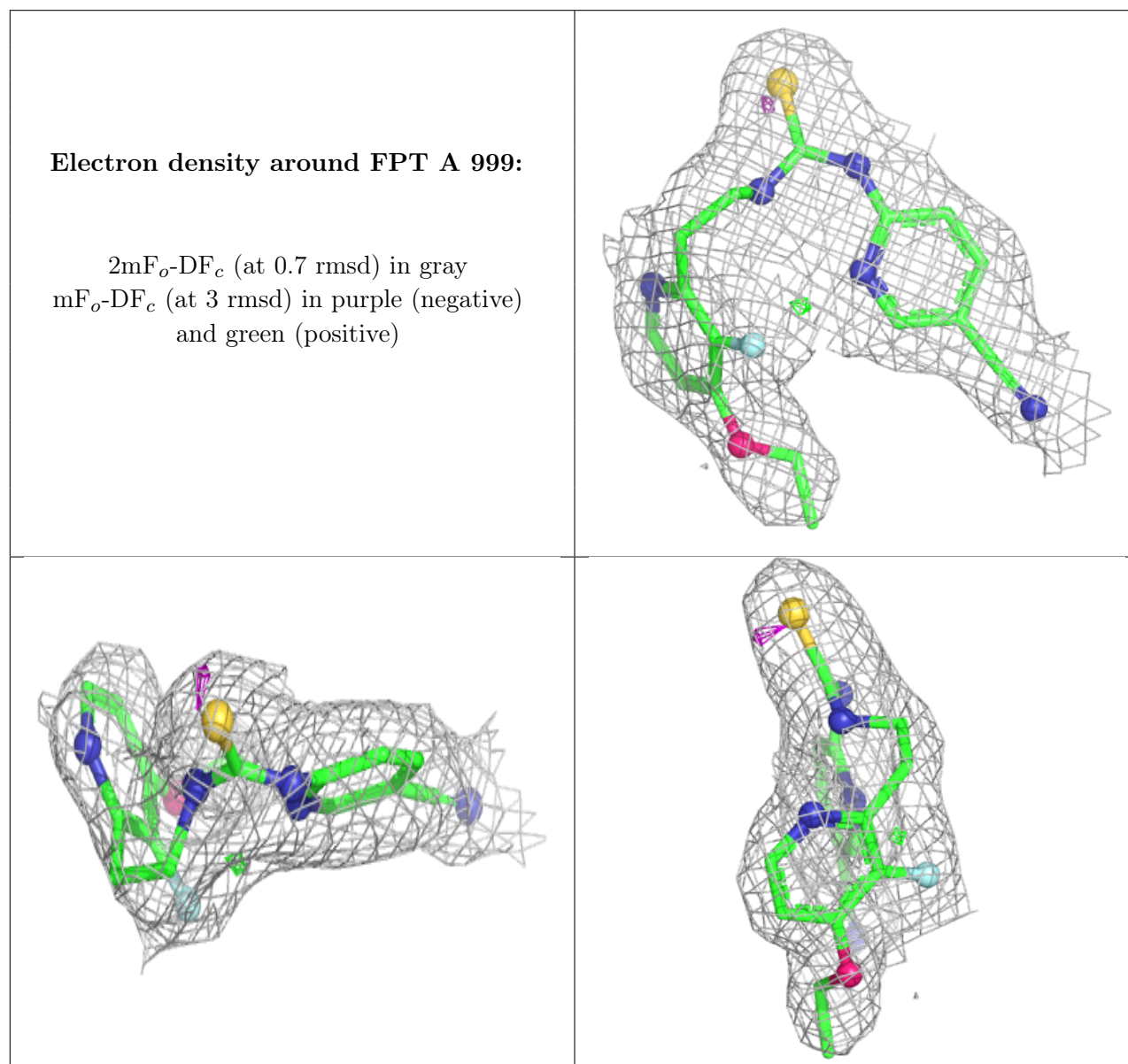
6.4 Ligands [i](#)

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
3	FPT	A	999	24/24	0.93	0.10	36,45,66,67	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.