



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 03:11 pm BST

PDB ID : 2QE2  
Title : Structure of HCV NS5B Bound to an Anthranilic Acid Inhibitor  
Authors : Chopra, R.; Svenson, K.; Bard, J.  
Deposited on : 2007-06-22  
Resolution : 2.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

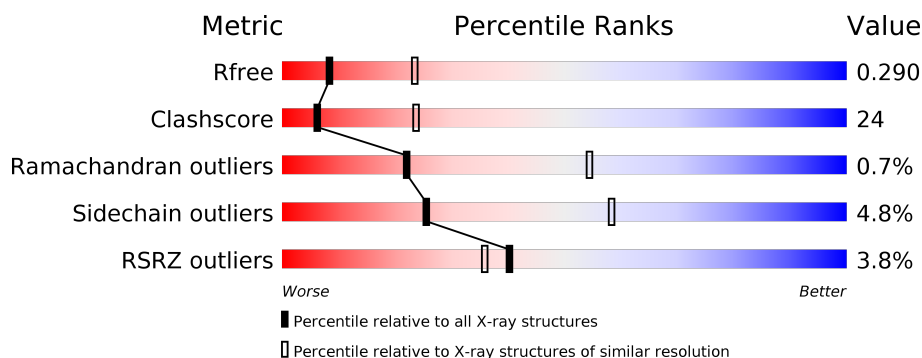
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	578	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>35%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	578	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>34%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8193 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.

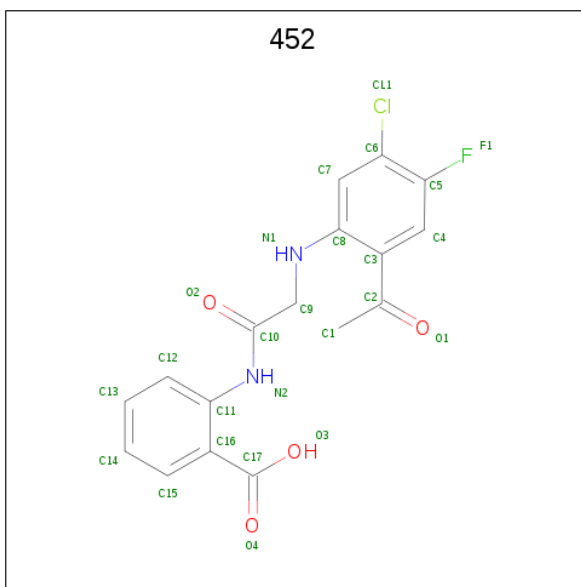
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4065	2567	721	748	29			
1	B	523	Total	C	N	O	S	0	0	0
			4078	2573	725	751	29			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	572	SER	-	EXPRESSION TAG	UNP Q99AU2
A	573	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	574	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	575	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	576	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	577	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	578	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	571	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	572	SER	-	EXPRESSION TAG	UNP Q99AU2
B	573	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	574	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	575	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	576	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	577	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	578	HIS	-	EXPRESSION TAG	UNP Q99AU2

- Molecule 2 is 2-{[N-(2-ACETYL-5-CHLORO-4-FLUOROPHENYL)GLYCYL]AMINO}BE NZOIC ACID (three-letter code: 452) (formula: C<sub>17</sub>H<sub>14</sub>ClFN<sub>2</sub>O<sub>4</sub>).

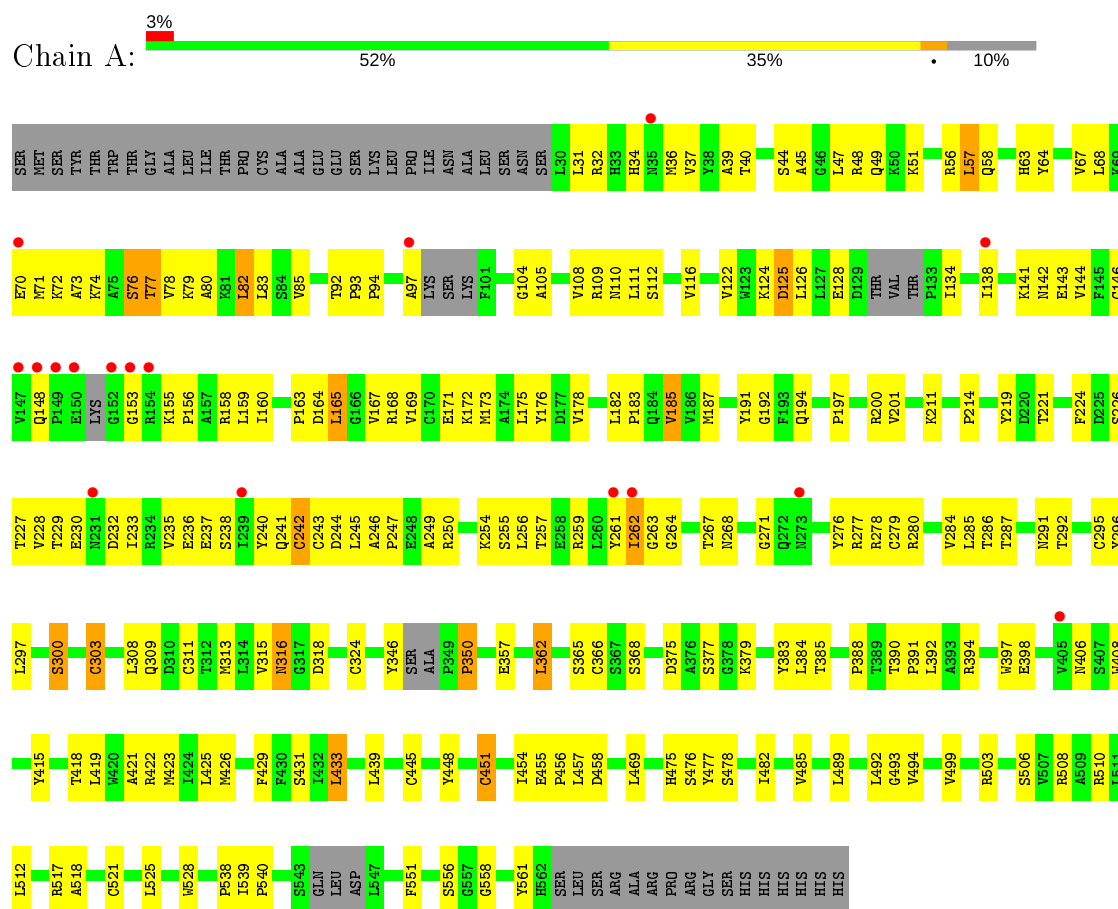


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			25	17	1	1	2	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			25	17	1	1	2	4		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: RNA-directed RNA polymerase



I482	L384	G290	N291	T292	L293	Y296	L297	S300	A301	A302	C303	R304	L308	Q309	D310	C311	T312	H313	L314	V315	N316	G317	D318	R319	L320	V321	V322	L323	C324	E325	F339	N343	Y346	SER	ALA	P349	P350	D359	L362	S365	C366	S367	S368	H374	S377	G378	K379	R380	Y383
V485	T385	G291	T292	F224	L293	Y296	L297	S300	A301	A302	C303	R304	L308	Q309	D310	C311	T312	H313	L314	V315	N316	G317	D318	R319	L320	V321	V322	L323	C324	E325	F339	N343	Y346	SER	ALA	P349	P350	D359	L362	S365	C366	S367	S368	H374	S377	G378	K379	R380	Y383
P495	P388	G292	T293	F224	L293	Y296	L297	S300	A301	A302	C303	R304	L308	Q309	D310	C311	T312	H313	L314	V315	N316	G317	D318	R319	L320	V321	V322	L323	C324	E325	F339	N343	Y346	SER	ALA	P349	P350	D359	L362	S365	C366	S367	S368	H374	S377	G378	K379	R380	Y383
P496	P389	G293	T294	F225	L294	Y297	L298	S301	A302	A303	C304	R305	L309	Q310	D311	C312	T313	H314	L315	V316	N317	G318	D319	R320	L321	V322	V323	L324	C325	E326	F340	N344	Y347	SER	ALA	P350	P351	D360	L363	S366	C367	S368	H375	S378	G379	K380	Y384		
V499	L392	G294	T295	F226	L295	Y298	L299	S302	A303	A304	C305	R306	L310	Q311	D312	C313	T314	H315	L316	V317	N318	G319	D320	R321	L322	V323	V324	L325	C326	E327	F341	N345	Y348	SER	ALA	P351	P352	D361	L364	S367	C368	S369	H376	S379	G380	K381	Y385		
R503	A393	G295	T296	F227	L296	Y299	L300	S303	A304	A305	C306	R307	L311	Q312	D313	C314	T315	H316	L317	V318	N319	G320	D321	R322	L323	V324	V325	L326	C327	E328	F342	N346	Y349	SER	ALA	P352	P353	D362	L365	S368	C369	S370	H377	S380	G381	K382	Y386		
W528	W397	G296	T297	F228	L297	Y300	L301	S304	A305	A306	C307	R308	L312	Q313	D314	C315	T316	H317	L318	V319	N320	G321	D322	R323	L324	V325	V326	L327	C328	E329	F343	N347	Y350	SER	ALA	P353	P354	D363	L366	S369	C370	S371	H378	S381	G382	K383	Y387		
P538	E398	G297	T298	F229	L298	Y301	L302	S305	A306	A307	C308	R309	L313	Q314	D315	C316	T317	H318	L319	V320	N321	G322	D323	R324	L325	V326	V327	L328	C329	E330	F344	N348	Y351	SER	ALA	P354	P355	D364	L367	S370	C371	S372	H379	S382	G383	K384	Y388		
A542	T403	G298	T299	F230	L299	Y302	L303	S306	A307	A308	C309	R310	L314	Q315	D316	C317	T318	H319	L320	V321	N322	G323	D324	R325	L326	V327	V328	L329	C330	E331	F345	N349	Y352	SER	ALA	P355	P356	D365	L368	S371	C372	S373	H380	S383	G384	K385	Y389		
S543	V405	G299	T300	F231	L300	Y303	L304	S307	A308	A309	C310	R311	L315	Q316	D317	C318	T319	H320	L321	V322	N323	G324	D325	R326	L327	V328	V329	L330	C331	E332	F346	N350	Y353	SER	ALA	P356	P357	D366	L369	S372	C373	S374	H381	S384	G385	K386	Y390		
GLN	M406	G300	T301	F232	L301	Y304	L305	S308	A309	A310	C311	R312	L316	Q317	D318	C319	T320	H321	L322	V323	N324	G325	D326	R327	L328	V329	V330	L331	C332	E333	F347	N351	Y354	SER	ALA	P357	P358	D367	L370	S373	C374	S375	H382	S385	G386	K387	Y391		
LEU	S407	G301	T302	F233	L302	Y305	L306	S309	A310	A311	C312	R313	L317	Q318	D319	C320	T321	H322	L323	V324	N325	G326	D327	R328	L329	V330	V331	L332	C333	E334	F348	N352	Y355	SER	ALA	P358	P359	D368	L371	S374	C375	S376	H383	S386	G387	K388	Y392		
ASP	W408	G302	T303	F234	L303	Y306	L307	S310	A311	A312	C313	R314	L318	Q319	D320	C321	T322	H323	L324	V325	N326	G327	D328	R329	L330	V331	V332	L333	C334	E335	F349	N353	Y356	SER	ALA	P359	P360	D369	L372	S375	C376	S377	H384	S387	G388	K389	Y393		
L547	Y415	G303	T304	F235	L304	Y307	L308	S311	A312	A313	C314	R315	L319	Q320	D321	C322	T323	H324	L325	V326	N327	G328	D329	R330	L331	V332	V333	L334	C335	E336	F350	N354	Y357	SER	ALA	P360	P361	D370	L373	S376	C377	S378	H385	S388	G389	K390	Y394		
F551	T418	G304	T305	F236	L305	Y308	L309	S312	A313	A314	C315	R316	L320	Q321	D322	C323	T324	H325	L326	V327	N328	G329	D330	R331	L332	V333	V334	L335	C336	E337	F351	N355	Y358	SER	ALA	P361	P362	D371	L374	S377	C378	S379	H386	S389	G390	K391	Y395		
S556	L419	G305	T306	F237	L306	Y309	L310	S313	A314	A315	C316	R317	L321	Q322	D323	C324	T325	H326	L327	V328	N329	G330	D331	R332	L333	V334	V335	L336	C337	E338	F352	N356	Y359	SER	ALA	P362	P363	D372	L375	S378	C379	S380	H387	S390	G391	K392	Y396		
G558	R422	G306	T307	F238	L307	Y310	L311	S314	A315	A316	C317	R318	L322	Q323	D324	C325	T326	H327	L328	V329	N330	G331	D332	R333	L334	V335	V336	L337	C338	E339	F353	N357	Y360	SER	ALA	P363	P364	D373	L376	S379	C380	S381	H388	S391	G392	K393	Y397		
D559	M423	G307	T308	F239	L308	Y311	L312	S315	A316	A317	C318	R319	L323	Q324	D325	C326	T327	H328	L329	V330	N331	G332	D333	R334	L335	V336	V337	L338	C339	E340	F354	N358	Y361	SER	ALA	P364	P365	D374	L377	S380	C381	S382	H389	S392	G393	K394	Y398		
I560	L425	G308	T309	F240	L309	Y312	L313	S316	A317	A318	C319	R320	L324	Q325	D326	C327	T328	H329	L330	V331	N332	G333	D334	R335	L336	V337	V338	L339	C340	E341	F355	N359	Y362	SER	ALA	P365	P366	D375	L378	S381	C382	S383	H390	S393	G394	K395	Y399		
Y561	L425	G309	T310	F241	L310	Y313	L314	S317	A318	A319	C320	R321	L325	Q326	D327	C328	T329	H330	L331	V332	N333	G334	D335	R336	L337	V338	V339	L340	C341	E342	F356	N360	Y363	SER	ALA	P366	P367	D376	L379	S382	C383	S384	H391	S394	G395	K396	Y400		
H562	F429	G310	T311	F242	L311	Y314	L315	S318	A319	A320	C321	R322	L326	Q327	D328	C329	T330	H331	L332	V333	N334	G335	D336	R337	L338	V339	V340	L341	C342	E343	F357	N361	Y364	SER	ALA	P367	P368	D377	L380	S383	C384	S385	H392	S395	G396	K397	Y401		
SER	F430	G311	T312	F243	L312	Y315	L316	S319	A320	A321	C322	R323	L327	Q328	D329	C330	T331	H332	L333	V334	N335	G336	D337	R338	L339	V340	V341	L342	C343	E344	F358	N362	Y365	SER	ALA	P368	P369	D378	L381	S384	C385	S386	H393	S396	G397	K398	Y402		
LEU	S431	G312	T313	F244	L313	Y316	L317	S320	A321	A322	C323	R324	L328	Q329	D330	C331	T332	H333	L334	V335	N336	G337	D338	R339	L340	V341	V342	L343	C344	E345	F359	N363	Y366	SER	ALA	P369	P370	D379	L382	S385	C386	S387	H394	S397	G398	K399	Y403		
SER	I432	G313	T314	F245	L314	Y317	L318	S321	A322	A323	C324	R325	L329	Q330	D331	C332	T333	H334	L335	V336	N337	G338	D339	R340	L341	V342	V343	L344	C345	E346	F360	N364	Y367	SER	ALA	P370	P371	D380	L383	S386	C387	S388	H395	S398	G399	K400	Y404		
ARG	L433	G314	T315	F246	L315	Y318	L319	S322	A323	A324	C325	R326	L330	Q331	D332	C333	T334	H335	L336	V337	N338	G339	D340	R341	L342	V343	V344	L345	C346	E347	F361	N365	Y368	SER	ALA	P371	P372	D381	L384	S387	C388	S389	H396	S399	G400	K401	Y405		
ARG	L439	G315	T316	F247	L316	Y319	L320	S323	A324	A325	C326	R327	L331	Q332	D333	C334	T335	H336	L337	V338	N339	G340	D341	R342	L343	V344	V345	L346	C347	E348	F362	N366	Y369	SER	ALA	P372	P373	D382	L385	S388	C389	S390	H397	S400	G401	K402	Y406		
PRO	L439	G316	T317	F248	L317	Y320	L321	S324	A325	A326	C327	R328	L332	Q333	D334	C335	T336	H337	L338	V339	N340	G341	D342	R343	L344	V345	V346	L347	C348	E349	F363	N367	Y370	SER	ALA	P373	P374	D383	L386	S389	C390	S391	H398	S401	G402	K403	Y407		
ARG	C445	G317	T318	F249	L318	Y321	L322	S325	A326	A327	C328	R329	L333	Q334	D335	C336	T337	H338	L339	V340	N341	G342	D343	R344	L345	V346	V347	L348	C349	E350	F364	N368	Y371	SER	ALA	P374	P375	D384	L387	S390	C391	S392	H399	S402	G403	K404	Y408		
GLY	C445	G318	T319	F250	L319	Y322	L323	S326	A327	A328	C329	R330	L334	Q335	D336	C337	T338	H339	L340	V341	N342	G343	D344	R345	L346	V347	V348	L349	C350	E351	F365	N369	Y372	SER	ALA	P375	P376	D385	L388	S391	C392	S393	H400	S403	G404	K405	Y409		
SER	Y448	G319	T320	F251	L320	Y323	L324	S327	A328	A329	C330	R331	L335	Q336	D337	C338	T339	H340	L341	V342	N343	G344	D345	R346	L347	V348	V349	L350	C351	E352	F366	N370	Y373	SER	ALA	P376	P377	D386	L389	S392	C393	S394	H401	S404	G405	K406	Y410		
HIS	Y448	G320	T321	F252	L321	Y324	L325	S328	A329	A330	C331	R332	L336	Q337	D338	C339	T340	H341	L342	V343	N344	G345	D346	R347	L348	V349	V350	L351	C352	E353	F367	N371	Y374	SER	ALA	P377	P378	D387	L390	S393	C394	S395	H402	S405	G406	K407	Y411		
HIS	C451	G321	T322	F253	L322	Y325	L326	S329	A330	A331	C332	R333	L337	Q338	D339	C340	T341	H342	L343	V344	N345	G346	D347	R348	L349	V350	V351	L352	C353	E354	F368	N372	Y375	SER	ALA	P378	P379	D388	L391	S									

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.83Å 70.88Å 251.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 2.90 49.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.77-2.90) 99.0 (49.14-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.279 , 0.296 0.272 , 0.290	Depositor DCC
$R_{free}$ test set	2495 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 21.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 452

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	0.48	0/4151	0.77	2/5622 (0.0%)
1	B	0.51	1/4166 (0.0%)	0.80	9/5643 (0.2%)
All	All	0.49	1/8317 (0.0%)	0.78	11/11265 (0.1%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	LYS	C-O	-6.71	1.10	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	LYS	N-CA-C	6.45	128.42	111.00
1	A	558	GLY	N-CA-C	-5.78	98.66	113.10
1	B	558	GLY	N-CA-C	-5.67	98.92	113.10
1	B	99	SER	N-CA-C	-5.62	95.83	111.00
1	B	101	PHE	N-CA-C	5.62	126.17	111.00
1	B	100	LYS	CA-C-N	-5.49	105.12	117.20
1	B	101	PHE	C-N-CA	-5.37	111.02	122.30
1	B	98	LYS	N-CA-C	5.33	125.41	111.00
1	B	99	SER	C-N-CA	-5.26	108.55	121.70
1	B	148	GLN	N-CA-C	5.25	125.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	LYS	Mainchain

## 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	4065	0	4071	204	0
1	B	4078	0	4084	198	0
2	A	25	0	13	0	0
2	B	25	0	13	0	0
All	All	8193	0	8181	400	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 24.

All (400) 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:261:TYR:HE1	1:A:284:VAL:HG11	1.17	1.06
1:B:230:GLU:HB3	1:B:262:ILE:HD11	1.39	1.03
1:A:254:LYS:HE3	1:B:254:LYS:HE3	1.42	0.97
1:B:377:SER:HB2	1:B:379:LYS:HG3	1.45	0.96
1:A:230:GLU:HB3	1:A:262:ILE:HD11	1.48	0.94
1:B:175:LEU:HD11	1:B:261:TYR:HE2	1.32	0.92
1:A:221:THR:HG1	1:A:224:PHE:HD1	0.93	0.91
1:A:261:TYR:CE1	1:A:284:VAL:HG11	2.09	0.87
1:B:44:SER:HB2	1:B:47:LEU:HD12	1.57	0.86
1:A:377:SER:HB2	1:A:379:LYS:HG3	1.59	0.85
1:A:309:GLN:O	1:A:324:CYS:HB2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TYR:O	1:A:194:GLN:HG2	1.79	0.82
1:A:163:PRO:HB2	1:A:167:VAL:HB	1.64	0.79
1:B:191:TYR:O	1:B:194:GLN:HG2	1.82	0.79
1:B:74:LYS:O	1:B:77:THR:HB	1.83	0.79
1:B:163:PRO:HB2	1:B:167:VAL:HB	1.64	0.79
1:B:71:MET:CE	1:B:297:LEU:HB2	2.13	0.78
1:A:76:SER:HA	1:A:242:CYS:O	1.83	0.78
1:A:79:LYS:HA	1:A:244:ASP:HB3	1.65	0.78
1:A:44:SER:HB2	1:A:47:LEU:HD12	1.66	0.77
1:A:394:ARG:O	1:A:398:GLU:HG3	1.84	0.77
1:A:74:LYS:O	1:A:77:THR:HB	1.84	0.77
1:B:175:LEU:HD13	1:B:286:THR:CG2	2.14	0.77
1:B:230:GLU:HB3	1:B:262:ILE:CD1	2.14	0.76
1:B:221:THR:HG1	1:B:224:PHE:HD1	1.30	0.76
1:B:309:GLN:O	1:B:324:CYS:HB2	1.86	0.76
1:A:171:GLU:OE1	1:A:284:VAL:HG12	1.84	0.76
1:B:303:CYS:SG	1:B:308:LEU:HD11	2.26	0.75
1:A:230:GLU:HB3	1:A:262:ILE:CD1	2.16	0.75
1:B:79:LYS:HA	1:B:244:ASP:HB3	1.68	0.75
1:A:303:CYS:SG	1:A:308:LEU:HD11	2.28	0.74
1:A:126:LEU:HA	1:A:259:ARG:NH1	2.02	0.74
1:B:245:LEU:HB2	1:B:250:ARG:HE	1.53	0.74
1:B:63:HIS:O	1:B:67:VAL:HG23	1.87	0.74
1:A:141:LYS:HG3	1:A:160:ILE:CG1	2.18	0.73
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.70	0.73
1:A:232:ASP:O	1:A:236:GLU:HG3	1.89	0.73
1:B:175:LEU:HD13	1:B:286:THR:HG23	1.68	0.73
1:A:175:LEU:HD13	1:A:286:THR:CG2	2.18	0.72
1:A:175:LEU:HD11	1:A:261:TYR:HE2	1.55	0.72
1:B:230:GLU:CB	1:B:262:ILE:HD11	2.17	0.72
1:B:71:MET:HE2	1:B:297:LEU:HB2	1.71	0.72
1:A:261:TYR:HE1	1:A:284:VAL:CG1	1.99	0.71
1:B:80:ALA:HB3	1:B:245:LEU:CD2	2.20	0.71
1:B:122:VAL:O	1:B:126:LEU:HB2	1.89	0.71
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.73	0.70
1:A:230:GLU:CB	1:A:262:ILE:HD11	2.19	0.70
1:A:201:VAL:HG22	1:A:384:LEU:HG	1.73	0.70
1:B:141:LYS:HG3	1:B:160:ILE:CG1	2.21	0.69
1:A:182:LEU:HB3	1:A:183:PRO:HD3	1.74	0.69
1:B:448:TYR:CE2	1:B:551:PHE:HD1	2.11	0.69
1:A:80:ALA:HB3	1:A:245:LEU:CD2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HB3	1:B:183:PRO:HD3	1.74	0.69
1:B:126:LEU:HA	1:B:259:ARG:NH1	2.07	0.69
1:B:175:LEU:CD1	1:B:261:TYR:HE2	2.06	0.69
1:B:76:SER:HA	1:B:242:CYS:O	1.93	0.68
1:A:175:LEU:HD13	1:A:286:THR:HG23	1.73	0.68
1:B:94:PRO:HG3	1:B:109:ARG:HH11	1.58	0.67
1:B:149:PRO:O	1:B:150:GLU:HB2	1.93	0.67
1:B:232:ASP:O	1:B:236:GLU:HG3	1.94	0.67
1:B:237:GLU:HG3	1:B:257:THR:HG21	1.76	0.67
1:A:485:VAL:O	1:A:489:LEU:HG	1.95	0.67
1:A:141:LYS:CG	1:A:160:ILE:HD11	2.25	0.66
1:B:148:GLN:O	1:B:151:LYS:HA	1.95	0.66
1:A:122:VAL:O	1:A:126:LEU:HB2	1.96	0.66
1:B:175:LEU:HD11	1:B:261:TYR:CE2	2.23	0.66
1:B:67:VAL:HG21	1:B:301:ALA:HB2	1.76	0.66
1:A:264:GLY:HA2	1:A:276:TYR:CZ	2.31	0.66
1:B:365:SER:O	1:B:366:CYS:HB2	1.96	0.66
1:B:388:PRO:O	1:B:392:LEU:HG	1.95	0.66
1:A:141:LYS:HG2	1:A:160:ILE:HD11	1.76	0.65
1:A:128:GLU:OE2	1:B:69:LYS:HE2	1.96	0.65
1:A:245:LEU:HB2	1:A:250:ARG:HE	1.61	0.65
1:A:171:GLU:OE1	1:A:284:VAL:CG1	2.44	0.65
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.30	0.65
1:B:445:CYS:HB3	1:B:454:ILE:HD12	1.78	0.64
1:B:67:VAL:O	1:B:71:MET:HG2	1.97	0.64
1:B:68:LEU:CD1	1:B:72:LYS:HE3	2.26	0.64
1:B:68:LEU:HD11	1:B:72:LYS:HE3	1.79	0.64
1:B:170:CYS:HA	1:B:173:MET:HE3	1.79	0.64
1:B:126:LEU:HD21	1:B:256:LEU:HG	1.80	0.64
1:B:394:ARG:O	1:B:398:GLU:HG3	1.98	0.63
1:A:71:MET:CE	1:A:297:LEU:HB2	2.28	0.63
1:B:94:PRO:HG3	1:B:109:ARG:NH1	2.12	0.63
1:A:63:HIS:O	1:A:67:VAL:HG23	1.98	0.63
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.81	0.62
1:B:263:GLY:HA2	1:B:277:ARG:NH1	2.14	0.62
1:A:237:GLU:HG3	1:A:257:THR:HG21	1.82	0.62
1:B:296:TYR:O	1:B:300:SER:HB2	2.00	0.62
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.80	0.62
1:A:68:LEU:HG	1:A:72:LYS:HE3	1.82	0.61
1:A:197:PRO:O	1:A:201:VAL:HG23	2.00	0.61
1:A:263:GLY:HA3	1:A:277:ARG:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TRP:HB2	1:A:429:PHE:CE2	2.36	0.60
1:B:99:SER:C	1:B:101:PHE:N	2.49	0.60
1:B:141:LYS:CG	1:B:160:ILE:HD11	2.31	0.60
1:A:388:PRO:O	1:A:392:LEU:HG	2.01	0.60
1:B:141:LYS:HG2	1:B:160:ILE:HD11	1.83	0.59
1:B:419:LEU:HD23	1:B:477:TYR:CG	2.37	0.59
1:A:235:VAL:O	1:A:238:SER:HB3	2.03	0.59
1:A:448:TYR:CE2	1:A:551:PHE:HD1	2.20	0.59
1:A:224:PHE:CG	1:A:318:ASP:HB3	2.38	0.59
1:B:263:GLY:HA3	1:B:277:ARG:O	2.03	0.58
1:A:68:LEU:CG	1:A:72:LYS:HE3	2.32	0.58
1:A:68:LEU:HD11	1:A:72:LYS:HE3	1.83	0.58
1:B:201:VAL:HG22	1:B:384:LEU:HG	1.84	0.58
1:A:175:LEU:O	1:A:178:VAL:N	2.26	0.58
1:A:31:LEU:HA	1:A:494:VAL:HG12	1.85	0.58
1:B:309:GLN:HG2	1:B:325:GLU:HB2	1.85	0.58
1:A:68:LEU:CD1	1:A:72:LYS:HE3	2.34	0.58
1:A:72:LYS:HB3	1:A:242:CYS:SG	2.44	0.58
1:A:126:LEU:HD21	1:A:256:LEU:HG	1.85	0.58
1:A:219:TYR:CZ	1:A:350:PRO:HB3	2.38	0.58
1:B:408:TRP:HB2	1:B:429:PHE:CE2	2.39	0.58
1:A:105:ALA:O	1:A:109:ARG:HG3	2.03	0.58
1:A:175:LEU:HD11	1:A:261:TYR:CE2	2.38	0.57
1:A:56:ARG:NH1	1:A:279:CYS:HB3	2.19	0.57
1:A:257:THR:HA	1:A:261:TYR:HB2	1.86	0.57
1:A:264:GLY:HA2	1:A:276:TYR:CE1	2.39	0.57
1:A:246:ALA:O	1:A:249:ALA:HB3	2.05	0.57
1:A:78:VAL:HG21	1:A:185:VAL:HG21	1.86	0.57
1:B:237:GLU:HA	1:B:240:TYR:CD2	2.40	0.57
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.87	0.57
1:A:230:GLU:HB3	1:A:262:ILE:CG1	2.35	0.57
1:B:141:LYS:HE3	1:B:158:ARG:HB2	1.87	0.57
1:B:246:ALA:O	1:B:249:ALA:HB3	2.04	0.57
1:B:261:TYR:HE1	1:B:284:VAL:HG11	1.69	0.57
1:A:445:CYS:HB3	1:A:454:ILE:HD12	1.87	0.57
1:A:78:VAL:CG2	1:A:185:VAL:HG21	2.35	0.56
1:B:78:VAL:HG21	1:B:185:VAL:HG21	1.87	0.56
1:B:191:TYR:CD1	1:B:292:THR:HG21	2.39	0.56
1:B:264:GLY:HA2	1:B:276:TYR:CZ	2.41	0.56
1:A:192:GLY:HA3	1:A:316:ASN:OD1	2.05	0.56
1:B:175:LEU:HD13	1:B:286:THR:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.87	0.56
1:A:71:MET:HE3	1:A:297:LEU:HB2	1.88	0.56
1:A:83:LEU:HB2	1:A:173:MET:HA	1.88	0.56
1:A:58:GLN:HG2	1:A:346:TYR:O	2.06	0.56
1:A:263:GLY:HA2	1:A:277:ARG:NH1	2.21	0.56
1:A:56:ARG:HH12	1:A:279:CYS:HB3	1.70	0.56
1:B:415:TYR:O	1:B:418:THR:HG23	2.06	0.56
1:B:175:LEU:CD1	1:B:261:TYR:CE2	2.87	0.55
1:A:134:ILE:HG13	1:A:259:ARG:HB3	1.89	0.55
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.88	0.55
1:B:149:PRO:C	1:B:151:LYS:H	2.08	0.55
1:B:99:SER:O	1:B:100:LYS:C	2.44	0.55
1:B:398:GLU:OE1	1:B:408:TRP:HD1	1.89	0.55
1:A:433:LEU:HB3	1:A:439:LEU:HD23	1.88	0.55
1:A:489:LEU:HD22	1:A:494:VAL:CG2	2.37	0.55
1:B:191:TYR:HD1	1:B:292:THR:HG21	1.70	0.54
1:B:221:THR:OG1	1:B:224:PHE:HD1	1.88	0.54
1:B:245:LEU:HD12	1:B:250:ARG:HG2	1.89	0.54
1:B:224:PHE:CG	1:B:318:ASP:HB3	2.42	0.54
1:A:365:SER:O	1:A:366:CYS:HB2	2.07	0.54
1:A:144:VAL:HG21	1:A:397:TRP:CD2	2.43	0.54
1:A:237:GLU:HA	1:A:240:TYR:CD2	2.42	0.54
1:B:40:THR:O	1:B:142:ASN:HA	2.06	0.54
1:B:108:VAL:HG21	1:B:165:LEU:HD21	1.89	0.54
1:A:40:THR:O	1:A:142:ASN:HA	2.06	0.54
1:B:80:ALA:HB3	1:B:245:LEU:HD23	1.90	0.54
1:B:48:ARG:HA	1:B:51:LYS:HD3	1.90	0.54
1:A:419:LEU:HD23	1:A:477:TYR:CG	2.42	0.53
1:B:423:MET:HG2	1:B:528:TRP:CZ3	2.44	0.53
1:A:165:LEU:O	1:A:169:VAL:HG23	2.09	0.53
1:B:170:CYS:HA	1:B:173:MET:CE	2.38	0.53
1:A:32:ARG:HB2	1:A:493:GLY:O	2.09	0.53
1:A:200:ARG:HD3	1:A:384:LEU:CD1	2.39	0.53
1:A:284:VAL:O	1:A:287:THR:HG22	2.08	0.52
1:B:58:GLN:HG2	1:B:346:TYR:O	2.09	0.52
1:B:48:ARG:CG	1:B:159:LEU:HG	2.40	0.52
1:B:144:VAL:HG21	1:B:397:TRP:CD2	2.45	0.52
1:A:241:GLN:HE22	1:A:250:ARG:HA	1.73	0.52
1:B:469:LEU:HD11	1:B:538:PRO:HA	1.91	0.52
1:A:241:GLN:HE22	1:A:250:ARG:CA	2.23	0.52
1:B:219:TYR:CZ	1:B:350:PRO:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HB3	1:B:242:CYS:SG	2.49	0.52
1:B:44:SER:CB	1:B:47:LEU:HD12	2.34	0.52
1:B:83:LEU:O	1:B:173:MET:HG2	2.10	0.52
1:A:423:MET:HG2	1:A:528:TRP:CZ3	2.45	0.51
1:A:499:VAL:HG12	1:A:503:ARG:NE	2.26	0.51
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.75	0.51
1:A:219:TYR:HE2	1:A:221:THR:HG22	1.73	0.51
1:A:303:CYS:SG	1:A:308:LEU:HD21	2.50	0.51
1:A:475:HIS:O	1:A:476:SER:HB2	2.09	0.51
1:A:56:ARG:NH1	1:A:226:SER:O	2.44	0.51
1:A:236:GLU:OE2	1:A:280:ARG:NH2	2.39	0.51
1:B:85:VAL:HG11	1:B:116:VAL:HG13	1.93	0.51
1:B:141:LYS:HG3	1:B:160:ILE:HG12	1.91	0.51
1:B:224:PHE:HE2	1:B:291:ASN:HA	1.76	0.51
1:A:224:PHE:CB	1:A:318:ASP:HB3	2.41	0.51
1:A:141:LYS:HG3	1:A:160:ILE:HG12	1.92	0.51
1:B:39:ALA:HB2	1:B:144:VAL:HG22	1.93	0.51
1:B:105:ALA:O	1:B:109:ARG:HG3	2.11	0.50
1:A:255:SER:O	1:A:259:ARG:HG3	2.11	0.50
1:B:478:SER:O	1:B:482:ILE:HG13	2.11	0.50
1:B:237:GLU:OE1	1:B:241:GLN:HG3	2.11	0.50
1:B:211:LYS:HB2	1:B:214:PRO:HB3	1.94	0.50
1:A:406:ASN:HD22	1:A:406:ASN:H	1.60	0.50
1:A:48:ARG:CG	1:A:159:LEU:HG	2.41	0.50
1:B:200:ARG:HD3	1:B:384:LEU:CD1	2.42	0.49
1:A:44:SER:CB	1:A:47:LEU:HD12	2.41	0.49
1:B:78:VAL:CG2	1:B:185:VAL:HG21	2.42	0.49
1:B:68:LEU:HA	1:B:71:MET:HG3	1.93	0.49
1:A:56:ARG:HD3	1:A:226:SER:O	2.11	0.49
1:B:475:HIS:O	1:B:476:SER:HB2	2.11	0.49
1:A:246:ALA:HB3	1:A:249:ALA:HB2	1.94	0.49
1:B:408:TRP:CB	1:B:429:PHE:CE2	2.95	0.49
1:A:224:PHE:O	1:A:228:VAL:HG23	2.12	0.49
1:A:191:TYR:HD1	1:A:292:THR:HG21	1.78	0.49
1:A:82:LEU:CD1	1:A:249:ALA:HB2	2.43	0.49
1:A:126:LEU:HA	1:A:259:ARG:HH12	1.74	0.49
1:A:31:LEU:HD21	1:A:34:HIS:HA	1.93	0.49
1:A:451:CYS:HB3	1:A:561:TYR:HD1	1.78	0.49
1:B:422:ARG:NH2	1:B:528:TRP:HB3	2.28	0.49
1:B:264:GLY:HA2	1:B:276:TYR:CE1	2.47	0.49
1:A:39:ALA:HB2	1:A:144:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HA	1:A:240:TYR:HD2	1.78	0.48
1:B:390:THR:HB	1:B:391:PRO:HD3	1.95	0.48
1:A:224:PHE:HE2	1:A:291:ASN:HA	1.78	0.48
1:B:377:SER:C	1:B:379:LYS:H	2.17	0.48
1:A:200:ARG:HD3	1:A:384:LEU:HD11	1.95	0.48
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.94	0.48
1:B:237:GLU:OE1	1:B:241:GLN:CG	2.62	0.48
1:A:141:LYS:HG3	1:A:160:ILE:HD11	1.94	0.48
1:A:47:LEU:HB2	1:A:156:PRO:HB3	1.95	0.48
1:A:408:TRP:CB	1:A:429:PHE:CE2	2.96	0.48
1:B:182:LEU:HD21	1:B:293:LEU:HD21	1.95	0.48
1:A:233:ILE:O	1:A:236:GLU:HB2	2.14	0.48
1:A:246:ALA:O	1:A:249:ALA:N	2.46	0.48
1:A:455:GLU:O	1:A:458:ASP:HB2	2.13	0.48
1:A:48:ARG:HA	1:A:51:LYS:HD3	1.95	0.48
1:B:125:ASP:OD1	1:B:259:ARG:NH2	2.43	0.48
1:B:175:LEU:O	1:B:178:VAL:HG12	2.13	0.48
1:B:66:ASP:HB3	1:B:304:ARG:HH12	1.78	0.48
1:A:383:TYR:HE2	1:A:385:THR:HB	1.79	0.48
1:A:398:GLU:OE1	1:A:408:TRP:HD1	1.97	0.48
1:B:230:GLU:HB3	1:B:262:ILE:CG1	2.42	0.48
1:B:419:LEU:HD11	1:B:485:VAL:HG11	1.96	0.48
1:A:80:ALA:HB3	1:A:245:LEU:HD23	1.95	0.48
1:A:303:CYS:SG	1:A:308:LEU:CD1	3.01	0.48
1:A:415:TYR:O	1:A:418:THR:HG23	2.13	0.48
1:A:296:TYR:O	1:A:300:SER:HB2	2.13	0.47
1:A:56:ARG:HE	1:A:229:THR:HG22	1.78	0.47
1:A:191:TYR:CD1	1:A:292:THR:HG21	2.49	0.47
1:B:284:VAL:HG23	1:B:287:THR:HB	1.94	0.47
1:A:243:CYS:O	1:A:245:LEU:HG	2.14	0.47
1:A:85:VAL:HG11	1:A:116:VAL:HG13	1.97	0.47
1:B:339:PHE:O	1:B:343:MET:HG2	2.15	0.47
1:B:47:LEU:HB2	1:B:156:PRO:HB3	1.97	0.47
1:B:56:ARG:HG3	1:B:56:ARG:HH11	1.80	0.47
1:B:126:LEU:HA	1:B:259:ARG:HH11	1.80	0.47
1:B:141:LYS:HG3	1:B:160:ILE:HD11	1.97	0.47
1:B:284:VAL:O	1:B:287:THR:HG22	2.15	0.47
1:A:124:LYS:O	1:A:128:GLU:HG3	2.15	0.46
1:A:398:GLU:OE2	1:A:406:ASN:HA	2.15	0.46
1:B:257:THR:HA	1:B:261:TYR:HB2	1.96	0.46
1:A:383:TYR:CE2	1:A:385:THR:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PRO:HB2	1:B:167:VAL:CB	2.40	0.46
1:B:233:ILE:O	1:B:236:GLU:HB2	2.15	0.46
1:B:398:GLU:OE2	1:B:406:ASN:HA	2.16	0.46
1:A:422:ARG:NH2	1:A:528:TRP:HB3	2.30	0.46
1:B:176:TYR:HA	1:B:285:LEU:HD21	1.96	0.46
1:B:149:PRO:C	1:B:151:LYS:N	2.67	0.46
1:A:110:ASN:O	1:A:111:LEU:HB2	2.15	0.46
1:A:141:LYS:HG3	1:A:160:ILE:CD1	2.45	0.46
1:A:97:ALA:O	1:A:168:ARG:NH2	2.48	0.46
1:A:31:LEU:HD22	1:A:37:VAL:HG21	1.98	0.46
1:B:192:GLY:HA3	1:B:316:ASN:OD1	2.15	0.46
1:A:506:SER:O	1:A:510:ARG:HG3	2.16	0.46
1:A:94:PRO:HG3	1:A:109:ARG:NH1	2.31	0.46
1:A:78:VAL:HB	1:A:243:CYS:SG	2.56	0.45
1:B:303:CYS:SG	1:B:308:LEU:CD1	3.02	0.45
1:A:94:PRO:HG3	1:A:109:ARG:HH11	1.81	0.45
1:B:237:GLU:CG	1:B:257:THR:HG21	2.45	0.45
1:B:84:SER:OG	1:B:87:GLU:HG3	2.16	0.45
1:A:56:ARG:HD3	1:A:227:THR:HA	1.97	0.45
1:A:377:SER:C	1:A:379:LYS:H	2.19	0.45
1:A:366:CYS:C	1:A:368:SER:H	2.20	0.45
1:A:377:SER:CB	1:A:379:LYS:HG3	2.36	0.45
1:A:489:LEU:HD22	1:A:494:VAL:HG21	1.97	0.45
1:A:499:VAL:CG1	1:A:503:ARG:HE	2.29	0.45
1:B:39:ALA:HA	1:B:143:GLU:O	2.16	0.45
1:A:245:LEU:HD12	1:A:250:ARG:HG2	1.99	0.45
1:A:263:GLY:HA2	1:A:277:ARG:CZ	2.47	0.45
1:B:75:ALA:C	1:B:77:THR:H	2.20	0.45
1:B:165:LEU:O	1:B:169:VAL:HG23	2.17	0.45
1:A:126:LEU:HA	1:A:259:ARG:HH11	1.78	0.45
1:B:108:VAL:CG2	1:B:165:LEU:HD21	2.46	0.45
1:B:469:LEU:HD11	1:B:538:PRO:CA	2.46	0.45
1:B:78:VAL:HB	1:B:243:CYS:SG	2.57	0.45
1:A:292:THR:HG23	1:A:315:VAL:HG12	1.97	0.45
1:A:313:MET:HE3	1:A:313:MET:HB2	1.82	0.45
1:A:56:ARG:NH2	1:A:278:ARG:O	2.49	0.45
1:A:141:LYS:HE3	1:A:158:ARG:HB2	1.99	0.44
1:A:221:THR:OG1	1:A:224:PHE:HD1	1.75	0.44
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.52	0.44
1:A:70:GLU:O	1:A:73:ALA:HB3	2.17	0.44
1:B:175:LEU:O	1:B:179:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:O	1:B:249:ALA:N	2.48	0.44
1:A:176:TYR:HA	1:A:285:LEU:HD21	1.99	0.44
1:B:465:ARG:NH1	1:B:543:SER:HA	2.32	0.44
1:A:92:THR:HA	1:A:93:PRO:HD3	1.80	0.44
1:B:125:ASP:OD1	1:B:125:ASP:C	2.56	0.44
1:B:313:MET:HE3	1:B:313:MET:HB2	1.68	0.44
1:A:303:CYS:SG	1:A:308:LEU:CG	3.05	0.44
1:B:419:LEU:C	1:B:419:LEU:HD12	2.38	0.44
1:A:182:LEU:O	1:A:185:VAL:N	2.47	0.44
1:A:175:LEU:HD13	1:A:286:THR:HG21	1.94	0.44
1:A:36:MET:O	1:A:146:CYS:HA	2.17	0.44
1:A:421:ALA:O	1:A:426:MET:HG3	2.18	0.44
1:A:457:LEU:HB3	1:A:517:ARG:HB3	2.00	0.44
1:B:56:ARG:HD2	1:B:229:THR:HG22	2.00	0.44
1:A:224:PHE:CB	1:A:318:ASP:CB	2.96	0.44
1:B:155:LYS:HA	1:B:156:PRO:HD3	1.82	0.44
1:B:163:PRO:HB3	1:B:167:VAL:HG21	1.99	0.44
1:B:179:VAL:HG12	1:B:289:CYS:CB	2.47	0.44
1:B:383:TYR:CE2	1:B:385:THR:HB	2.53	0.44
1:B:224:PHE:CB	1:B:318:ASP:HB3	2.48	0.44
1:B:55:ASP:OD1	1:B:56:ARG:N	2.51	0.44
1:A:163:PRO:CB	1:A:167:VAL:HB	2.42	0.44
1:B:261:TYR:HE1	1:B:284:VAL:CG1	2.31	0.44
1:B:179:VAL:HG12	1:B:289:CYS:HB2	2.00	0.44
1:B:255:SER:O	1:B:259:ARG:HG3	2.18	0.43
1:A:182:LEU:HB3	1:A:183:PRO:CD	2.47	0.43
1:B:45:ALA:O	1:B:49:GLN:HG3	2.18	0.43
1:A:469:LEU:HD11	1:A:538:PRO:HA	2.00	0.43
1:B:406:ASN:HD22	1:B:406:ASN:H	1.66	0.43
1:A:518:ALA:O	1:A:521:CYS:HB2	2.19	0.43
1:B:183:PRO:HB3	1:B:187:MET:CE	2.48	0.43
1:B:433:LEU:HB3	1:B:439:LEU:HD23	1.99	0.43
1:A:408:TRP:HB2	1:A:429:PHE:CD2	2.54	0.43
1:B:542:ALA:O	1:B:543:SER:HB2	2.18	0.43
1:A:31:LEU:CD2	1:A:34:HIS:HA	2.49	0.43
1:A:439:LEU:HB3	1:A:457:LEU:HD21	2.01	0.43
1:A:56:ARG:HH21	1:A:229:THR:HA	1.83	0.43
1:A:478:SER:O	1:A:482:ILE:HG13	2.18	0.43
1:B:282:SER:O	1:B:287:THR:HG21	2.19	0.43
1:A:469:LEU:HD23	1:A:469:LEU:HA	1.88	0.43
1:B:141:LYS:HG3	1:B:160:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:PHE:CB	1:B:318:ASP:CB	2.97	0.43
1:B:408:TRP:HB2	1:B:429:PHE:CD2	2.53	0.43
1:A:267:THR:HG22	1:A:268:ASN:O	2.19	0.42
1:B:366:CYS:C	1:B:368:SER:H	2.21	0.42
1:A:419:LEU:C	1:A:419:LEU:HD12	2.39	0.42
1:B:126:LEU:HA	1:B:259:ARG:HH12	1.82	0.42
1:B:359:ASP:HB3	1:B:362:LEU:HD22	2.00	0.42
1:B:499:VAL:HG12	1:B:503:ARG:NE	2.34	0.42
1:A:71:MET:HE1	1:A:297:LEU:HB2	2.00	0.42
1:B:32:ARG:O	1:B:34:HIS:N	2.48	0.42
1:A:164:ASP:O	1:A:167:VAL:N	2.53	0.42
1:A:308:LEU:HD11	1:A:311:CYS:SG	2.59	0.42
1:A:155:LYS:HA	1:A:156:PRO:HD3	1.83	0.42
1:B:134:ILE:HG22	1:B:135:ASP:N	2.35	0.42
1:B:66:ASP:HB3	1:B:304:ARG:NH1	2.34	0.42
1:B:56:ARG:HE	1:B:229:THR:HG22	1.85	0.42
1:B:178:VAL:CG1	1:B:179:VAL:N	2.82	0.42
1:B:495:PRO:HA	1:B:496:PRO:HD3	1.90	0.42
1:A:183:PRO:HB3	1:A:187:MET:CE	2.50	0.42
1:A:39:ALA:HA	1:A:143:GLU:O	2.20	0.42
1:B:190:SER:HA	1:B:313:MET:O	2.19	0.42
1:B:315:VAL:HG22	1:B:320:LEU:CD1	2.50	0.42
1:A:390:THR:HB	1:A:391:PRO:HD3	2.02	0.42
1:A:237:GLU:OE1	1:A:241:GLN:CG	2.68	0.41
1:B:197:PRO:O	1:B:201:VAL:HG23	2.20	0.41
1:B:313:MET:HG2	1:B:322:VAL:HG22	2.02	0.41
1:A:148:GLN:HG3	1:A:153:GLY:O	2.20	0.41
1:B:196:SER:HA	1:B:551:PHE:CD1	2.55	0.41
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.90	0.41
1:A:224:PHE:CZ	1:A:295:CYS:HB2	2.56	0.41
1:A:68:LEU:HA	1:A:68:LEU:HD12	1.82	0.41
1:A:45:ALA:O	1:A:49:GLN:HG3	2.21	0.41
1:B:237:GLU:HG2	1:B:257:THR:OG1	2.20	0.41
1:A:125:ASP:OD1	1:A:125:ASP:C	2.59	0.41
1:A:539:ILE:HG23	1:A:540:PRO:HD2	2.01	0.41
1:B:172:LYS:HE2	1:B:559:ASP:O	2.20	0.41
1:A:104:GLY:O	1:A:108:VAL:HG23	2.21	0.41
1:A:146:CYS:SG	1:A:492:LEU:HD21	2.60	0.41
1:A:164:ASP:O	1:A:165:LEU:C	2.57	0.41
1:B:221:THR:OG1	1:B:224:PHE:CD1	2.69	0.41
1:B:456:PRO:C	1:B:458:ASP:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:GLU:OE2	1:A:362:LEU:HD23	2.21	0.41
1:B:36:MET:O	1:B:146:CYS:HA	2.21	0.41
1:B:374:HIS:CE1	1:B:380:ARG:HG3	2.56	0.41
1:B:64:TYR:CD2	1:B:64:TYR:C	2.94	0.41
1:B:61:ASP:C	1:B:63:HIS:N	2.73	0.41
1:A:172:LYS:HA	1:A:176:TYR:HB2	2.02	0.41
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.86	0.41
1:B:237:GLU:HA	1:B:240:TYR:HD2	1.84	0.41
1:B:451:CYS:HB3	1:B:561:TYR:HD1	1.85	0.41
1:B:455:GLU:O	1:B:458:ASP:HB2	2.21	0.41
1:B:56:ARG:NH1	1:B:56:ARG:HG3	2.35	0.40
1:A:508:ARG:O	1:A:512:LEU:HG	2.21	0.40
1:B:277:ARG:CZ	1:B:281:ALA:HB2	2.52	0.40
1:B:71:MET:HE2	1:B:297:LEU:CB	2.46	0.40
1:B:148:GLN:HG3	1:B:153:GLY:O	2.22	0.40
1:B:311:CYS:HA	1:B:324:CYS:HB3	2.03	0.40
1:A:375:ASP:OD1	1:A:377:SER:N	2.47	0.40
1:B:228:VAL:HG21	1:B:280:ARG:HB2	2.01	0.40
1:A:521:CYS:O	1:A:525:LEU:HB2	2.22	0.40
1:B:110:ASN:O	1:B:111:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/578 (88%)	466 (92%)	41 (8%)	2 (0%)	34	66
1	B	515/578 (89%)	464 (90%)	46 (9%)	5 (1%)	15	45
All	All	1024/1156 (89%)	930 (91%)	87 (8%)	7 (1%)	22	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	LYS
1	A	165	LEU
1	B	34	HIS
1	B	33	HIS
1	A	271	GLY
1	B	457	LEU
1	B	271	GLY

### 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	443/492 (90%)	420 (95%)	23 (5%)	23	55
1	B	444/492 (90%)	424 (96%)	20 (4%)	27	61
All	All	887/984 (90%)	844 (95%)	43 (5%)	25	58

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	64	TYR
1	A	76	SER
1	A	77	THR
1	A	82	LEU
1	A	112	SER
1	A	125	ASP
1	A	138	ILE
1	A	185	VAL
1	A	242	CYS
1	A	247	PRO
1	A	262	ILE
1	A	300	SER
1	A	303	CYS
1	A	316	ASN
1	A	350	PRO
1	A	362	LEU

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Mol	Chain	Res	Type
1	A	425	LEU
1	A	431	SER
1	A	433	LEU
1	A	451	CYS
1	A	456	PRO
1	A	556	SER
1	B	64	TYR
1	B	77	THR
1	B	82	LEU
1	B	112	SER
1	B	125	ASP
1	B	138	ILE
1	B	178	VAL
1	B	233	ILE
1	B	242	CYS
1	B	247	PRO
1	B	262	ILE
1	B	284	VAL
1	B	300	SER
1	B	303	CYS
1	B	316	ASN
1	B	350	PRO
1	B	425	LEU
1	B	431	SER
1	B	451	CYS
1	B	556	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	241	GLN
1	B	194	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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
2	452	A	579	-	24,26,26	2.63	13 (54%)	31,36,36	1.32	4 (12%)
2	452	B	579	-	24,26,26	2.65	13 (54%)	31,36,36	1.37	5 (16%)

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
2	452	A	579	-	-	0/13/17/17	0/2/2/2
2	452	B	579	-	-	0/13/17/17	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	452	C16-C17	5.53	1.52	1.47
2	B	579	452	C7-C8	4.78	1.47	1.39
2	A	579	452	C16-C11	4.41	1.46	1.40
2	A	579	452	C7-C8	4.18	1.46	1.39
2	B	579	452	C3-C8	4.15	1.47	1.41
2	B	579	452	C16-C17	4.15	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	452	C4-C5	4.13	1.44	1.37
2	B	579	452	C4-C3	3.96	1.46	1.39
2	B	579	452	C16-C11	3.96	1.46	1.40
2	B	579	452	C4-C5	3.70	1.44	1.37
2	A	579	452	C4-C3	3.65	1.45	1.39
2	B	579	452	C6-C5	3.33	1.43	1.38
2	A	579	452	C12-C11	3.29	1.45	1.39
2	A	579	452	C6-C5	3.23	1.43	1.38
2	B	579	452	C12-C11	2.88	1.44	1.39
2	A	579	452	C15-C16	2.86	1.44	1.40
2	B	579	452	C3-C2	2.73	1.54	1.48
2	A	579	452	C3-C8	2.70	1.45	1.41
2	B	579	452	C15-C16	2.70	1.44	1.40
2	B	579	452	C8-N1	2.66	1.44	1.37
2	B	579	452	C9-N1	2.44	1.49	1.45
2	B	579	452	C7-C6	2.41	1.42	1.38
2	A	579	452	C3-C2	2.24	1.53	1.48
2	A	579	452	C10-N2	2.22	1.40	1.35
2	A	579	452	C8-N1	2.19	1.43	1.37
2	A	579	452	C11-N2	2.09	1.45	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	452	C9-N1-C8	3.27	128.66	123.98
2	A	579	452	C9-N1-C8	2.99	128.26	123.98
2	B	579	452	F1-C5-C6	2.53	121.31	118.98
2	A	579	452	F1-C5-C6	2.34	121.14	118.98
2	B	579	452	O2-C10-N2	2.21	127.66	123.63
2	B	579	452	C15-C16-C17	-2.21	116.91	120.20
2	A	579	452	C8-C7-C6	2.16	123.50	120.05
2	B	579	452	C8-C7-C6	2.11	123.42	120.05
2	A	579	452	C4-C5-C6	-2.03	119.76	121.72

There are no chirality outliers.

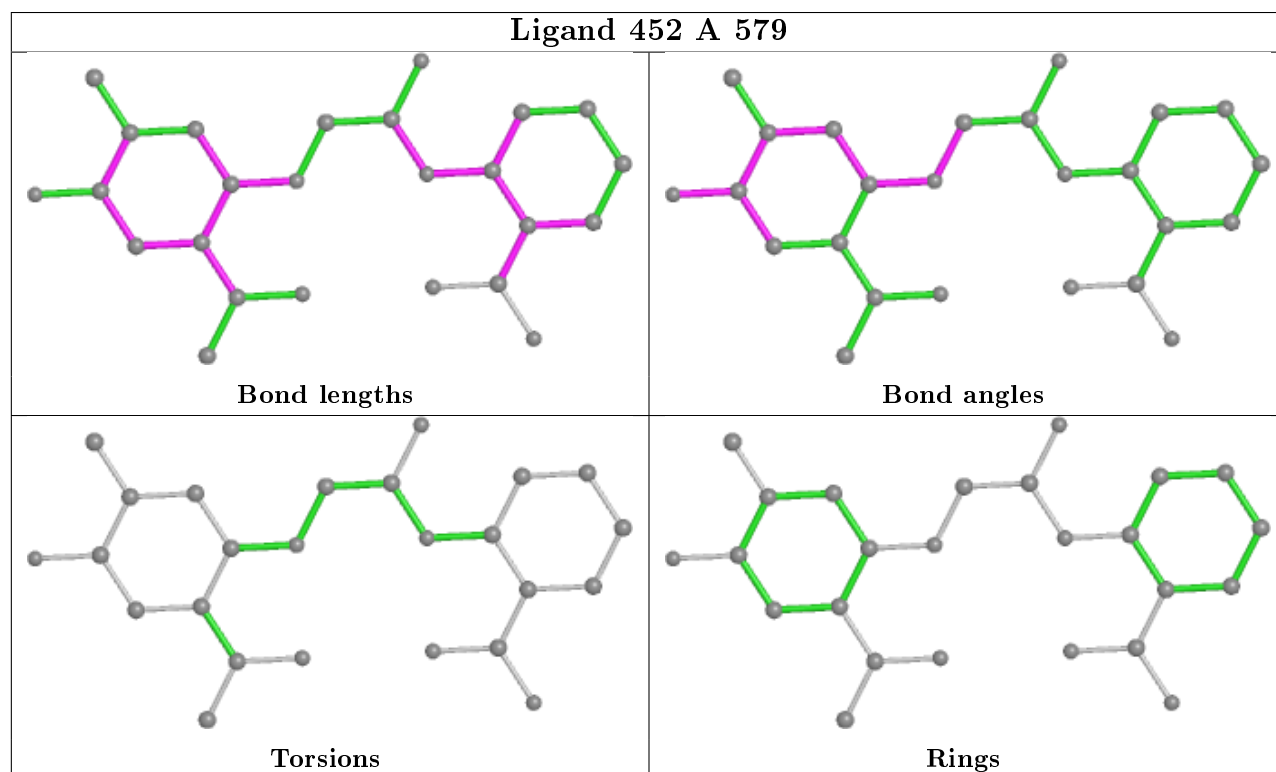
There are no torsion outliers.

There are no ring outliers.

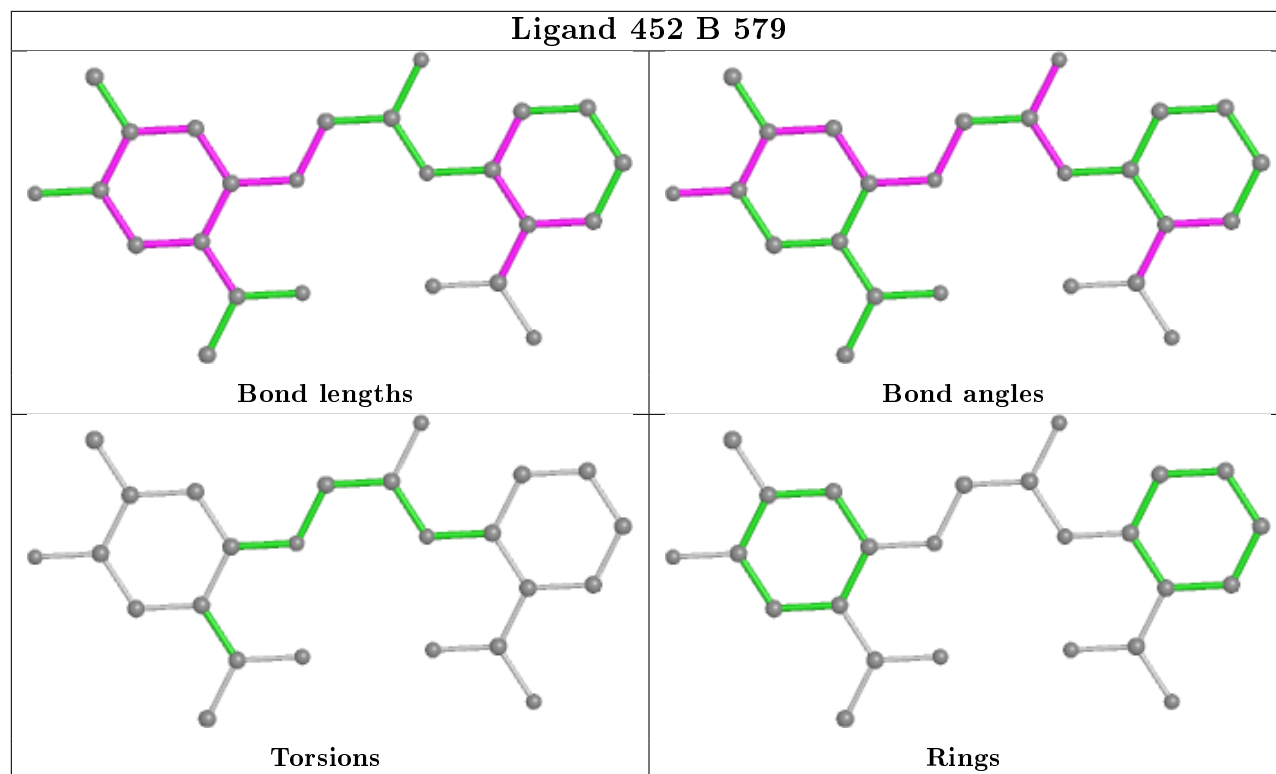
No monomer is involved in short contacts.

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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	521/578 (90%)	0.00	17 (3%)	46 41	18, 43, 77, 119	0
1	B	523/578 (90%)	0.03	23 (4%)	34 30	19, 43, 79, 115	0
All	All	1044/1156 (90%)	0.01	40 (3%)	40 36	18, 43, 78, 119	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	GLY	9.7
1	A	150	GLU	7.3
1	B	150	GLU	6.4
1	B	149	PRO	5.3
1	B	152	GLY	4.9
1	A	153	GLY	4.2
1	A	261	TYR	3.7
1	A	147	VAL	3.6
1	A	273	ASN	3.5
1	A	138	ILE	3.4
1	A	35	ASN	3.4
1	B	405	VAL	3.3
1	A	148	GLN	3.2
1	B	60	LEU	3.2
1	B	153	GLY	3.1
1	B	35	ASN	3.1
1	B	262	ILE	3.0
1	B	51	LYS	2.8
1	B	286	THR	2.7
1	B	235	VAL	2.7
1	B	80	ALA	2.6
1	A	262	ILE	2.6
1	B	273	ASN	2.6
1	A	70	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	174	ALA	2.5
1	A	154	ARG	2.4
1	B	161	VAL	2.4
1	B	403	THR	2.4
1	A	405	VAL	2.3
1	A	97	ALA	2.3
1	B	134	ILE	2.3
1	B	265	PRO	2.2
1	B	279	CYS	2.2
1	A	239	ILE	2.1
1	A	149	PRO	2.1
1	B	47	LEU	2.1
1	B	148	GLN	2.1
1	B	36	MET	2.0
1	B	59	VAL	2.0
1	A	231	ASN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

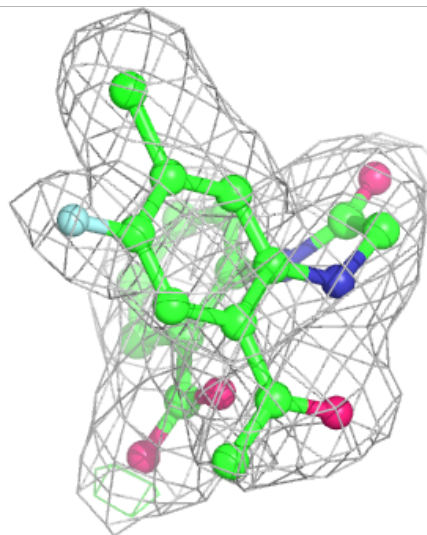
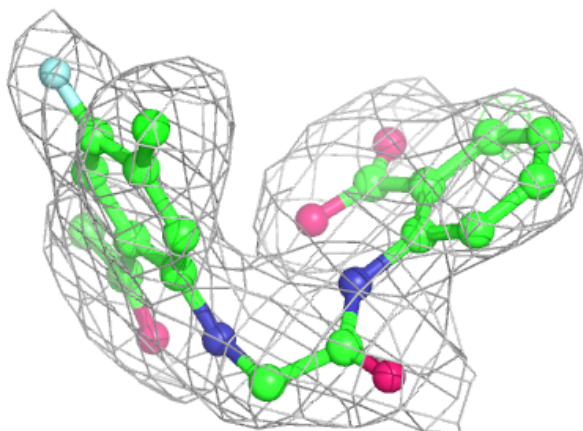
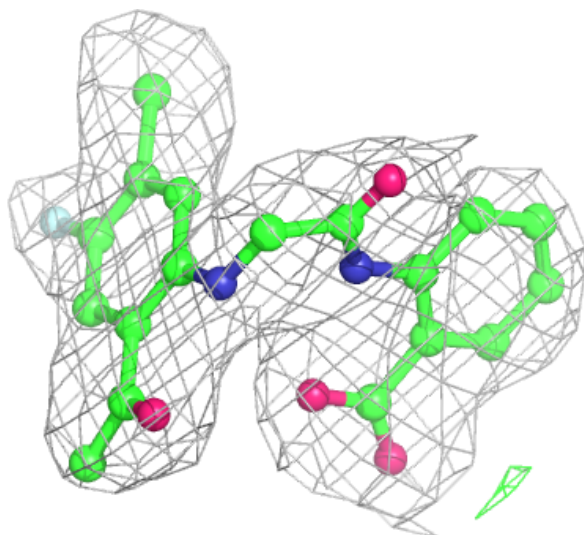
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	452	A	579	25/25	0.93	0.16	22,32,37,42	0
2	452	B	579	25/25	0.93	0.15	22,31,37,39	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.

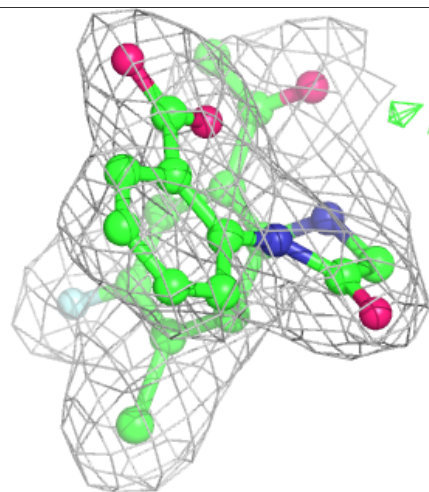
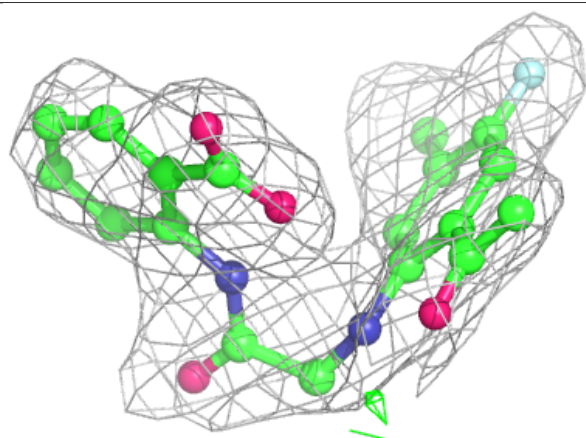
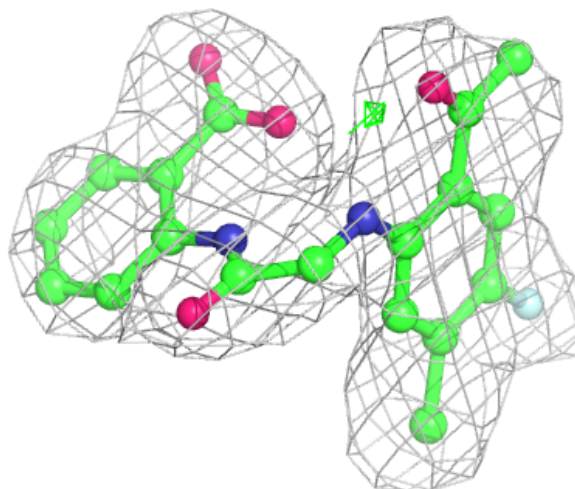
**Electron density around 452 A 579:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 452 B 579:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.