



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:00 AM UTC

PDB ID : 1MMJ / pdb_00001mmj
Title : Porcine pancreatic elastase complexed with a potent peptidyl inhibitor,
FR136706
Authors : Kinoshita, T.
Deposited on : 2002-09-04
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

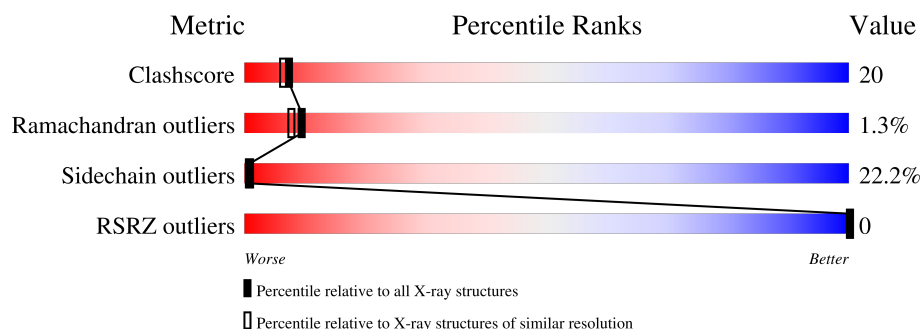
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	N	240	18% 44% 25% 13%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2137 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 elastase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	N	240	1822	1135	329	348	10	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



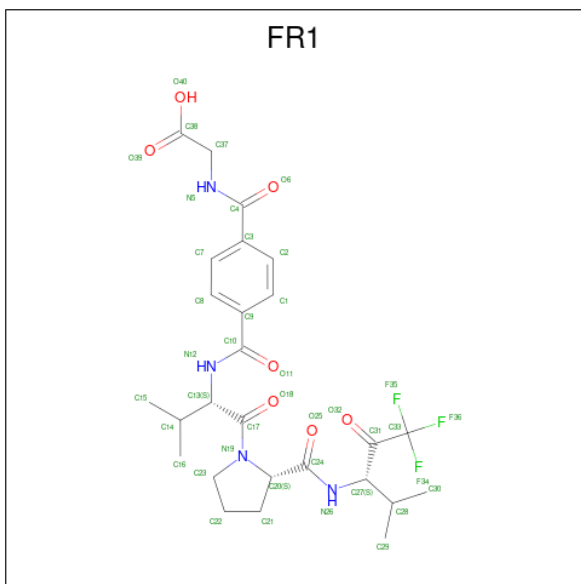
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	N	1	5	4	1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	N	1	1	1	0	0

- Molecule 4 is 2-[4-[[[(S)-1-[[[(S)-2-[[[(RS)-3,3,3-TRIFLUORO-1-ISOPROPYL-2-OXOP

ROPYL]AMINOCARBONYL]PYRROLIDIN-1-YL-]CARBONYL]-2-METHYLPROPYL]AMINOCARBONYL]BENZOYLAMINO]ACETIC ACID (CCD ID: FR1) (formula: $C_{26}H_{33}F_3N_4O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	N	1	Total	C	F	N	O	0	0
			40	26	3	4	7		

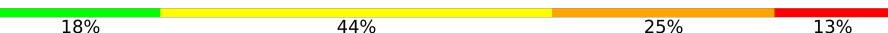
- Molecule 5 is water.

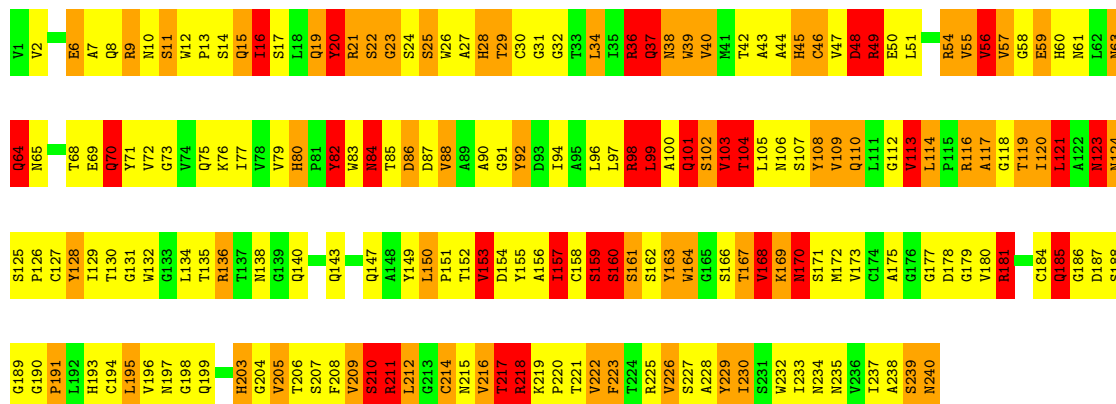
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	269	Total	O	0	0
			269	269		

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: elastase 1

Chain N: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.29Å 58.31Å 75.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 46.15 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 95.4 (46.15-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.40Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.215 , 0.241 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	6.0	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2137	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% 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: CA, FR1, SO4

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	N	2.65	119/1862 (6.4%)	3.24	300/2543 (11.8%)

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	N	0	26

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	193	HIS	CE1-NE2	12.48	1.45	1.32
1	N	203	HIS	CE1-NE2	12.27	1.44	1.32
1	N	31	GLY	N-CA	10.66	1.55	1.44
1	N	12	TRP	N-CA	9.95	1.57	1.46
1	N	234	ASN	CA-C	9.80	1.65	1.52
1	N	203	HIS	ND1-CE1	9.46	1.42	1.32
1	N	211	ARG	NE-CZ	9.31	1.43	1.33
1	N	177	GLY	CA-C	9.28	1.64	1.51
1	N	126	PRO	CA-C	8.92	1.61	1.52
1	N	57	VAL	CA-C	8.70	1.63	1.52
1	N	203	HIS	CG-CD2	8.67	1.45	1.35
1	N	194	CYS	CA-C	8.38	1.63	1.52
1	N	45	HIS	ND1-CE1	8.34	1.40	1.32
1	N	116	ARG	NE-CZ	8.28	1.42	1.33
1	N	235	ASN	N-CA	8.26	1.56	1.46
1	N	32	GLY	CA-C	8.24	1.60	1.51
1	N	193	HIS	CG-ND1	-8.22	1.29	1.38
1	N	128	TYR	CA-C	8.11	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	29	THR	CA-C	7.99	1.63	1.52
1	N	226	VAL	C-N	7.82	1.44	1.33
1	N	83	TRP	CA-C	7.79	1.62	1.52
1	N	193	HIS	ND1-CE1	7.74	1.40	1.32
1	N	98	ARG	NE-CZ	7.69	1.41	1.33
1	N	180	VAL	CA-C	7.66	1.61	1.52
1	N	108	TYR	CA-C	7.64	1.62	1.52
1	N	230	ILE	C-N	7.56	1.44	1.33
1	N	119	THR	CA-C	-7.53	1.43	1.52
1	N	204	GLY	N-CA	7.51	1.56	1.45
1	N	233	ILE	CA-CB	7.25	1.62	1.54
1	N	114	LEU	CA-CB	-7.20	1.43	1.53
1	N	150	LEU	CA-C	7.11	1.60	1.52
1	N	138	ASN	C-N	7.04	1.43	1.33
1	N	90	ALA	C-N	6.92	1.44	1.33
1	N	181	ARG	NE-CZ	6.91	1.40	1.33
1	N	210	SER	N-CA	6.86	1.54	1.45
1	N	85	THR	CA-C	-6.73	1.43	1.52
1	N	163	TYR	N-CA	6.72	1.54	1.46
1	N	99	LEU	C-N	-6.71	1.24	1.34
1	N	230	ILE	CB-CG1	6.69	1.66	1.53
1	N	232	TRP	CD2-CE2	6.68	1.52	1.41
1	N	43	ALA	N-CA	6.63	1.54	1.46
1	N	60	HIS	C-N	6.59	1.42	1.33
1	N	25	SER	N-CA	6.57	1.54	1.46
1	N	37	GLN	CA-C	-6.56	1.43	1.52
1	N	197	ASN	N-CA	6.55	1.55	1.46
1	N	36	ARG	NE-CZ	6.54	1.40	1.33
1	N	21	ARG	N-CA	6.46	1.54	1.46
1	N	190	GLY	C-N	6.45	1.41	1.33
1	N	58	GLY	N-CA	6.43	1.54	1.45
1	N	7	ALA	CA-CB	6.41	1.63	1.53
1	N	186	GLY	N-CA	6.39	1.55	1.44
1	N	46	CYS	CA-CB	-6.31	1.43	1.53
1	N	206	THR	CA-CB	-6.29	1.43	1.53
1	N	156	ALA	C-N	6.24	1.41	1.33
1	N	21	ARG	NE-CZ	6.20	1.39	1.33
1	N	38	ASN	C-N	6.15	1.41	1.33
1	N	121	LEU	N-CA	6.13	1.53	1.46
1	N	97	LEU	C-N	6.10	1.42	1.33
1	N	209	VAL	CA-CB	-6.08	1.46	1.54
1	N	42	THR	C-O	6.08	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	235	ASN	C-N	5.99	1.41	1.33
1	N	70	GLN	CA-C	-5.94	1.45	1.52
1	N	92	TYR	N-CA	-5.92	1.37	1.46
1	N	15	GLN	N-CA	5.92	1.53	1.46
1	N	143	GLN	C-O	-5.92	1.16	1.24
1	N	217	THR	N-CA	5.90	1.53	1.46
1	N	207	SER	CA-C	-5.89	1.47	1.52
1	N	116	ARG	N-CA	5.89	1.53	1.46
1	N	113	VAL	CA-C	5.88	1.59	1.52
1	N	195	LEU	C-N	-5.86	1.25	1.33
1	N	143	GLN	CA-CB	5.86	1.63	1.53
1	N	185	GLN	N-CA	5.84	1.53	1.45
1	N	160	SER	CA-C	5.82	1.60	1.52
1	N	68	THR	CA-CB	-5.82	1.45	1.53
1	N	34	LEU	CB-CG	-5.78	1.41	1.53
1	N	30	CYS	CA-C	-5.78	1.45	1.52
1	N	226	VAL	CA-CB	5.76	1.62	1.54
1	N	31	GLY	CA-C	5.74	1.60	1.52
1	N	140	GLN	N-CA	5.73	1.53	1.45
1	N	124	ASN	CA-CB	-5.72	1.44	1.53
1	N	80	HIS	N-CA	5.72	1.52	1.45
1	N	29	THR	CB-OG1	5.69	1.52	1.43
1	N	177	GLY	N-CA	5.69	1.53	1.45
1	N	116	ARG	CA-CB	5.67	1.62	1.53
1	N	217	THR	CB-OG1	-5.62	1.34	1.43
1	N	156	ALA	CA-C	5.60	1.60	1.52
1	N	75	GLN	CA-C	5.57	1.60	1.52
1	N	59	GLU	C-N	5.51	1.41	1.33
1	N	214	CYS	CA-C	-5.50	1.46	1.52
1	N	180	VAL	CA-CB	5.45	1.62	1.55
1	N	172	MET	SD-CE	5.43	1.93	1.79
1	N	49	ARG	NE-CZ	5.41	1.39	1.33
1	N	131	GLY	CA-C	5.41	1.57	1.51
1	N	206	THR	CA-C	5.39	1.59	1.52
1	N	91	GLY	CA-C	5.38	1.58	1.52
1	N	181	ARG	C-N	5.33	1.40	1.33
1	N	150	LEU	N-CA	5.28	1.52	1.46
1	N	49	ARG	N-CA	-5.27	1.39	1.45
1	N	54	ARG	NE-CZ	5.23	1.38	1.33
1	N	180	VAL	N-CA	5.20	1.50	1.46
1	N	212	LEU	CA-CB	-5.20	1.44	1.53
1	N	19	GLN	CA-C	5.19	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	215	ASN	N-CA	5.18	1.53	1.46
1	N	21	ARG	C-O	-5.18	1.17	1.24
1	N	54	ARG	CZ-NH2	-5.17	1.26	1.33
1	N	232	TRP	CA-C	5.14	1.59	1.52
1	N	205	VAL	CA-CB	5.13	1.60	1.54
1	N	212	LEU	CA-C	-5.12	1.45	1.52
1	N	45	HIS	CG-CD2	5.11	1.41	1.35
1	N	230	ILE	N-CA	5.09	1.52	1.46
1	N	152	THR	N-CA	5.07	1.52	1.46
1	N	113	VAL	N-CA	5.06	1.52	1.46
1	N	134	LEU	CA-CB	5.06	1.61	1.53
1	N	24	SER	N-CA	5.05	1.52	1.46
1	N	127	CYS	CA-C	5.05	1.58	1.52
1	N	15	GLN	CA-C	5.04	1.59	1.52
1	N	195	LEU	CA-C	5.01	1.59	1.52
1	N	123	ASN	CA-CB	-5.01	1.45	1.53
1	N	125	SER	C-N	5.01	1.38	1.33

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	103	VAL	N-CA-CB	-12.05	91.34	111.23
1	N	64	GLN	CA-CB-CG	11.96	138.01	114.10
1	N	48	ASP	CA-CB-CG	-11.73	100.87	112.60
1	N	22	SER	N-CA-CB	11.31	126.04	111.00
1	N	159	SER	N-CA-C	11.13	124.98	111.40
1	N	178	ASP	N-CA-C	11.09	126.31	113.01
1	N	169	LYS	N-CA-C	10.80	126.50	109.65
1	N	22	SER	CB-CA-C	-10.80	92.28	109.13
1	N	11	SER	N-CA-C	10.65	124.18	111.82
1	N	175	ALA	CA-C-N	10.56	130.84	121.86
1	N	175	ALA	C-N-CA	10.56	130.84	121.86
1	N	20	TYR	CA-C-O	10.44	133.68	121.46
1	N	218	ARG	CD-NE-CZ	-10.44	109.78	124.40
1	N	221	THR	CA-C-N	-10.38	107.11	122.68
1	N	221	THR	C-N-CA	-10.38	107.11	122.68
1	N	24	SER	N-CA-C	10.24	132.62	110.80
1	N	181	ARG	CA-CB-CG	10.23	134.57	114.10
1	N	212	LEU	CB-CA-C	-10.12	90.89	110.11
1	N	123	ASN	OD1-CG-ND2	-10.02	112.58	122.60
1	N	36	ARG	CD-NE-CZ	-9.98	110.43	124.40
1	N	86	ASP	N-CA-C	9.98	124.55	112.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	143	GLN	CB-CG-CD	-9.84	95.87	112.60
1	N	120	ILE	CA-CB-CG1	-9.76	93.81	110.40
1	N	116	ARG	CB-CG-CD	9.73	133.68	111.30
1	N	220	PRO	CB-CA-C	9.59	123.51	111.23
1	N	181	ARG	NE-CZ-NH2	9.53	127.78	119.20
1	N	48	ASP	N-CA-C	9.39	124.37	113.19
1	N	110	GLN	CG-CD-NE2	-9.33	102.40	116.40
1	N	157	ILE	N-CA-C	9.32	120.13	110.72
1	N	181	ARG	CD-NE-CZ	-9.26	111.43	124.40
1	N	94	ILE	CA-C-O	-9.25	112.27	120.96
1	N	96	LEU	CA-C-O	9.19	131.54	121.16
1	N	218	ARG	N-CA-C	9.13	124.06	113.38
1	N	63	ASN	CA-CB-CG	9.10	121.69	112.60
1	N	155	TYR	N-CA-C	9.09	122.33	111.33
1	N	238	ALA	N-CA-C	9.02	121.93	111.11
1	N	118	GLY	N-CA-C	8.99	126.84	115.42
1	N	166	SER	CA-C-N	-8.86	106.07	121.66
1	N	166	SER	C-N-CA	-8.86	106.07	121.66
1	N	14	SER	N-CA-CB	8.78	125.17	110.41
1	N	104	THR	CA-CB-CG2	-8.68	95.75	110.50
1	N	6	GLU	CB-CA-C	8.64	124.42	109.65
1	N	217	THR	CB-CA-C	-8.53	95.96	109.70
1	N	105	LEU	O-C-N	8.53	132.91	123.10
1	N	222	VAL	CA-CB-CG2	8.49	124.83	110.40
1	N	38	ASN	CB-CG-OD1	8.47	137.74	120.80
1	N	92	TYR	CA-C-N	-8.45	108.82	122.34
1	N	92	TYR	C-N-CA	-8.45	108.82	122.34
1	N	161	SER	N-CA-C	8.43	121.60	111.82
1	N	151	PRO	CA-C-N	-8.27	109.60	121.42
1	N	151	PRO	C-N-CA	-8.27	109.60	121.42
1	N	29	THR	CA-CB-CG2	8.26	124.55	110.50
1	N	38	ASN	CB-CG-ND2	-8.24	104.03	116.40
1	N	164	TRP	CA-C-O	8.18	129.18	119.28
1	N	239	SER	N-CA-C	8.11	121.22	111.82
1	N	197	ASN	OD1-CG-ND2	-8.09	114.51	122.60
1	N	163	TYR	CA-C-N	-8.09	107.75	122.38
1	N	163	TYR	C-N-CA	-8.09	107.75	122.38
1	N	228	ALA	CB-CA-C	-8.01	93.84	110.17
1	N	34	LEU	CD1-CG-CD2	-7.93	93.36	110.80
1	N	12	TRP	CB-CA-C	-7.92	100.48	111.41
1	N	181	ARG	NH1-CZ-NH2	-7.81	109.15	119.30
1	N	49	ARG	CA-C-N	-7.76	111.00	122.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	49	ARG	C-N-CA	-7.76	111.00	122.41
1	N	126	PRO	N-CA-CB	-7.75	97.10	103.30
1	N	135	THR	N-CA-C	7.75	122.57	113.20
1	N	218	ARG	CA-C-N	-7.71	113.06	123.46
1	N	218	ARG	C-N-CA	-7.71	113.06	123.46
1	N	113	VAL	N-CA-C	7.70	119.05	108.89
1	N	212	LEU	N-CA-CB	7.63	122.78	110.42
1	N	100	ALA	N-CA-CB	-7.61	98.48	110.28
1	N	106	ASN	CA-CB-CG	-7.57	105.03	112.60
1	N	17	SER	CA-C-N	-7.53	112.33	122.72
1	N	17	SER	C-N-CA	-7.53	112.33	122.72
1	N	31	GLY	N-CA-C	-7.51	100.71	112.58
1	N	90	ALA	N-CA-C	7.49	120.33	111.71
1	N	214	CYS	O-C-N	7.48	130.11	122.03
1	N	44	ALA	CB-CA-C	-7.47	96.80	110.63
1	N	157	ILE	CA-C-O	7.42	128.72	120.85
1	N	29	THR	CB-CA-C	-7.42	96.56	109.02
1	N	79	VAL	CG1-CB-CG2	-7.41	94.49	110.80
1	N	232	TRP	N-CA-C	7.41	119.35	111.28
1	N	72	VAL	CG1-CB-CG2	-7.36	94.61	110.80
1	N	63	ASN	CB-CG-ND2	-7.33	105.40	116.40
1	N	86	ASP	CA-CB-CG	-7.31	105.29	112.60
1	N	15	GLN	CG-CD-NE2	-7.28	105.49	116.40
1	N	108	TYR	N-CA-CB	-7.26	99.85	110.53
1	N	117	ALA	CA-C-N	-7.26	111.46	122.28
1	N	117	ALA	C-N-CA	-7.26	111.46	122.28
1	N	94	ILE	O-C-N	7.24	130.14	123.19
1	N	136	ARG	NE-CZ-NH1	-7.21	114.29	121.50
1	N	216	VAL	CA-C-N	-7.17	110.78	120.90
1	N	216	VAL	C-N-CA	-7.17	110.78	120.90
1	N	85	THR	N-CA-C	7.17	120.01	111.33
1	N	10	ASN	CA-C-N	-7.11	109.50	120.31
1	N	10	ASN	C-N-CA	-7.11	109.50	120.31
1	N	11	SER	CA-C-N	7.03	130.39	122.59
1	N	11	SER	C-N-CA	7.03	130.39	122.59
1	N	234	ASN	N-CA-CB	-7.02	99.48	109.94
1	N	36	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	N	110	GLN	CA-C-O	-6.95	113.55	121.40
1	N	188	SER	CB-CA-C	-6.94	98.64	109.61
1	N	203	HIS	CA-C-N	-6.94	107.80	121.41
1	N	203	HIS	C-N-CA	-6.94	107.80	121.41
1	N	233	ILE	N-CA-CB	6.94	118.19	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	22	SER	O-C-N	6.92	129.44	122.10
1	N	128	TYR	CA-C-N	-6.92	109.90	122.43
1	N	128	TYR	C-N-CA	-6.92	109.90	122.43
1	N	159	SER	CA-CB-OG	6.91	124.93	111.10
1	N	134	LEU	CD1-CG-CD2	6.88	125.93	110.80
1	N	9	ARG	CB-CA-C	-6.87	97.48	110.67
1	N	209	VAL	CG1-CB-CG2	6.85	125.86	110.80
1	N	225	ARG	CA-C-O	6.82	128.34	120.98
1	N	116	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	N	21	ARG	N-CA-C	6.68	119.92	109.96
1	N	63	ASN	CA-C-N	-6.68	108.78	121.54
1	N	63	ASN	C-N-CA	-6.68	108.78	121.54
1	N	14	SER	CB-CA-C	-6.61	96.80	109.95
1	N	103	VAL	CA-CB-CG1	6.60	121.62	110.40
1	N	56	VAL	CA-CB-CG2	6.56	121.55	110.40
1	N	114	LEU	CB-CG-CD2	6.56	130.38	110.70
1	N	24	SER	CA-C-N	-6.55	109.02	121.54
1	N	24	SER	C-N-CA	-6.55	109.02	121.54
1	N	36	ARG	NH1-CZ-NH2	-6.53	110.81	119.30
1	N	100	ALA	N-CA-C	6.52	119.38	111.82
1	N	83	TRP	CA-C-N	-6.50	113.61	122.77
1	N	83	TRP	C-N-CA	-6.50	113.61	122.77
1	N	47	VAL	CA-CB-CG1	-6.48	99.39	110.40
1	N	116	ARG	CD-NE-CZ	6.46	133.44	124.40
1	N	178	ASP	CA-CB-CG	6.44	119.04	112.60
1	N	193	HIS	CB-CA-C	-6.43	100.20	110.81
1	N	170	ASN	CA-CB-CG	6.41	119.01	112.60
1	N	55	VAL	CA-CB-CG1	6.40	121.29	110.40
1	N	61	ASN	CA-C-O	-6.40	113.40	120.38
1	N	198	GLY	CA-C-N	-6.39	112.38	122.73
1	N	198	GLY	C-N-CA	-6.39	112.38	122.73
1	N	157	ILE	CA-CB-CG2	6.39	121.36	110.50
1	N	70	GLN	N-CA-C	6.38	119.55	108.76
1	N	130	THR	CA-CB-OG1	6.35	119.12	109.60
1	N	70	GLN	CA-CB-CG	6.33	126.75	114.10
1	N	199	GLN	CA-C-N	-6.33	112.09	120.95
1	N	199	GLN	C-N-CA	-6.33	112.09	120.95
1	N	101	GLN	CG-CD-OE1	6.31	133.43	120.80
1	N	47	VAL	O-C-N	6.31	130.45	122.57
1	N	168	VAL	CA-CB-CG1	6.28	121.08	110.40
1	N	187	ASP	CA-CB-CG	-6.27	106.33	112.60
1	N	64	GLN	N-CA-C	6.25	124.12	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	143	GLN	CA-CB-CG	6.24	126.59	114.10
1	N	166	SER	CB-CA-C	-6.23	97.75	109.72
1	N	160	SER	N-CA-C	6.23	124.07	110.80
1	N	77	ILE	CA-C-O	-6.19	113.90	120.53
1	N	208	PHE	CA-C-O	6.18	127.69	120.89
1	N	51	LEU	CD1-CG-CD2	-6.18	97.20	110.80
1	N	132	TRP	N-CA-C	6.17	120.51	112.92
1	N	239	SER	O-C-N	6.15	129.84	122.27
1	N	214	CYS	CA-C-O	-6.15	114.57	120.90
1	N	49	ARG	N-CA-CB	-6.14	100.11	111.53
1	N	101	GLN	N-CA-C	-6.14	99.74	109.07
1	N	153	VAL	CA-CB-CG1	6.12	120.81	110.40
1	N	28	HIS	CA-C-N	-6.12	112.63	122.24
1	N	28	HIS	C-N-CA	-6.12	112.63	122.24
1	N	155	TYR	CB-CA-C	-6.11	100.30	110.68
1	N	16	ILE	CA-CB-CG1	6.08	120.74	110.40
1	N	20	TYR	CA-C-N	-6.08	112.02	121.02
1	N	20	TYR	C-N-CA	-6.08	112.02	121.02
1	N	40	VAL	CA-CB-CG2	6.07	120.72	110.40
1	N	87	ASP	N-CA-CB	-6.06	102.37	111.64
1	N	25	SER	CA-C-N	-6.04	113.11	122.59
1	N	25	SER	C-N-CA	-6.04	113.11	122.59
1	N	156	ALA	CA-C-N	-6.01	111.88	120.42
1	N	156	ALA	C-N-CA	-6.01	111.88	120.42
1	N	97	LEU	CB-CA-C	-6.00	100.91	110.14
1	N	101	GLN	CA-CB-CG	5.98	126.07	114.10
1	N	106	ASN	CB-CG-ND2	-5.98	107.42	116.40
1	N	223	PHE	CA-C-O	5.98	128.00	121.06
1	N	65	ASN	N-CA-C	5.97	119.26	110.30
1	N	189	GLY	CA-C-N	-5.97	112.50	121.87
1	N	189	GLY	C-N-CA	-5.97	112.50	121.87
1	N	73	GLY	N-CA-C	5.95	120.15	112.54
1	N	109	VAL	CG1-CB-CG2	5.94	123.87	110.80
1	N	120	ILE	CA-C-O	5.93	126.64	120.36
1	N	38	ASN	O-C-N	5.92	130.21	122.15
1	N	54	ARG	CA-C-N	-5.92	112.73	122.67
1	N	54	ARG	C-N-CA	-5.92	112.73	122.67
1	N	105	LEU	CA-C-N	5.88	132.77	121.54
1	N	105	LEU	C-N-CA	5.88	132.77	121.54
1	N	28	HIS	CA-CB-CG	5.88	119.68	113.80
1	N	29	THR	CA-CB-OG1	-5.87	100.79	109.60
1	N	216	VAL	N-CA-C	5.87	116.38	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	64	GLN	CA-C-O	5.85	128.88	120.51
1	N	99	LEU	CB-CA-C	-5.84	98.14	109.76
1	N	173	VAL	CA-C-N	-5.83	114.48	122.93
1	N	173	VAL	C-N-CA	-5.83	114.48	122.93
1	N	121	LEU	N-CA-C	5.83	118.91	110.28
1	N	222	VAL	CA-CB-CG1	5.81	120.27	110.40
1	N	239	SER	CB-CA-C	-5.80	99.54	110.67
1	N	140	GLN	CA-C-O	-5.77	114.69	121.44
1	N	238	ALA	CA-C-O	5.76	127.06	120.90
1	N	211	ARG	N-CA-C	5.74	119.90	113.01
1	N	217	THR	N-CA-C	5.73	118.32	110.24
1	N	44	ALA	CA-C-N	-5.71	110.53	121.94
1	N	44	ALA	C-N-CA	-5.71	110.53	121.94
1	N	101	GLN	CG-CD-NE2	-5.70	107.85	116.40
1	N	63	ASN	CB-CG-OD1	5.70	132.20	120.80
1	N	84	ASN	CB-CG-ND2	-5.70	107.85	116.40
1	N	225	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	N	16	ILE	O-C-N	5.67	129.33	123.04
1	N	6	GLU	CA-CB-CG	5.66	125.43	114.10
1	N	169	LYS	CA-C-N	-5.65	112.16	122.38
1	N	169	LYS	C-N-CA	-5.65	112.16	122.38
1	N	212	LEU	CA-C-N	-5.64	114.40	122.64
1	N	212	LEU	C-N-CA	-5.64	114.40	122.64
1	N	132	TRP	O-C-N	5.64	129.11	122.34
1	N	138	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	N	65	ASN	CB-CG-ND2	-5.64	107.94	116.40
1	N	69	GLU	CB-CA-C	5.62	119.02	109.53
1	N	188	SER	N-CA-C	5.62	118.21	110.35
1	N	155	TYR	O-C-N	-5.61	116.18	122.12
1	N	234	ASN	CA-C-O	5.57	126.86	120.90
1	N	232	TRP	CA-C-O	5.57	126.45	120.55
1	N	63	ASN	O-C-N	-5.56	114.72	121.83
1	N	172	MET	N-CA-CB	-5.55	102.60	111.43
1	N	203	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
1	N	209	VAL	CB-CA-C	-5.50	103.64	111.34
1	N	140	GLN	N-CA-C	5.49	118.04	109.52
1	N	107	SER	N-CA-C	5.48	119.69	112.89
1	N	173	VAL	CA-C-O	-5.47	114.56	120.36
1	N	172	MET	CA-C-O	-5.46	115.24	121.58
1	N	227	SER	N-CA-C	5.45	119.03	112.38
1	N	80	HIS	CA-C-N	-5.44	113.16	119.47
1	N	80	HIS	C-N-CA	-5.44	113.16	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	171	SER	N-CA-C	-5.43	106.69	113.15
1	N	56	VAL	CB-CA-C	5.43	118.04	110.99
1	N	58	GLY	CA-C-O	5.42	126.63	119.58
1	N	38	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	N	120	ILE	CA-CB-CG2	5.41	119.69	110.50
1	N	54	ARG	CG-CD-NE	-5.40	100.11	112.00
1	N	197	ASN	CB-CA-C	-5.39	103.60	112.06
1	N	27	ALA	CA-C-N	-5.38	113.36	121.05
1	N	27	ALA	C-N-CA	-5.38	113.36	121.05
1	N	25	SER	CB-CA-C	-5.36	99.75	110.42
1	N	223	PHE	CZ-CE2-CD2	-5.36	110.36	120.00
1	N	180	VAL	N-CA-CB	-5.34	107.26	111.64
1	N	69	GLU	CA-CB-CG	5.33	124.76	114.10
1	N	237	ILE	CA-C-N	5.32	127.73	120.54
1	N	237	ILE	C-N-CA	5.32	127.73	120.54
1	N	195	LEU	N-CA-CB	-5.32	101.20	109.87
1	N	123	ASN	N-CA-C	5.32	117.74	110.24
1	N	153	VAL	CA-CB-CG2	5.31	119.43	110.40
1	N	205	VAL	CA-C-O	5.31	126.21	120.53
1	N	199	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	N	99	LEU	CD1-CG-CD2	5.31	122.48	110.80
1	N	88	VAL	N-CA-CB	5.30	121.28	110.78
1	N	147	GLN	CA-C-O	-5.30	115.41	121.40
1	N	126	PRO	N-CA-C	5.30	118.82	110.50
1	N	230	ILE	N-CA-C	5.29	120.33	109.34
1	N	106	ASN	OD1-CG-ND2	5.28	127.88	122.60
1	N	181	ARG	N-CA-C	5.27	118.08	109.59
1	N	215	ASN	CA-CB-CG	-5.27	107.33	112.60
1	N	70	GLN	N-CA-CB	5.27	119.92	110.80
1	N	225	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	N	117	ALA	N-CA-C	5.25	121.99	110.80
1	N	205	VAL	N-CA-C	5.25	115.42	107.80
1	N	42	THR	CA-C-N	-5.25	114.32	122.09
1	N	42	THR	C-N-CA	-5.25	114.32	122.09
1	N	20	TYR	N-CA-C	5.24	118.13	109.85
1	N	47	VAL	N-CA-C	5.23	120.22	109.34
1	N	101	GLN	CA-C-O	-5.22	115.69	121.33
1	N	140	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	N	15	GLN	CG-CD-OE1	5.22	131.24	120.80
1	N	119	THR	CA-CB-CG2	5.21	119.36	110.50
1	N	107	SER	N-CA-CB	5.21	118.89	110.40
1	N	197	ASN	CB-CG-OD1	5.21	131.22	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	223	PHE	CE1-CZ-CE2	5.20	129.35	120.00
1	N	64	GLN	O-C-N	-5.18	115.69	122.59
1	N	46	CYS	N-CA-CB	5.18	118.52	110.44
1	N	150	LEU	N-CA-CB	-5.17	103.91	111.20
1	N	16	ILE	CA-C-N	-5.17	115.81	123.05
1	N	16	ILE	C-N-CA	-5.17	115.81	123.05
1	N	191	PRO	CA-C-O	5.16	128.69	122.19
1	N	184	CYS	CB-CA-C	-5.16	101.29	111.91
1	N	80	HIS	O-C-N	5.15	125.60	121.38
1	N	48	ASP	CA-C-O	5.13	127.12	118.91
1	N	112	GLY	CA-C-N	-5.12	114.59	121.66
1	N	112	GLY	C-N-CA	-5.12	114.59	121.66
1	N	103	VAL	O-C-N	-5.12	116.17	122.57
1	N	39	TRP	CD2-CE3-CZ3	-5.11	111.95	118.60
1	N	193	HIS	ND1-CG-CD2	5.09	111.19	106.10
1	N	147	GLN	CG-CD-OE1	5.08	130.97	120.80
1	N	37	GLN	CA-C-O	-5.08	112.46	119.12
1	N	75	GLN	CB-CA-C	5.07	119.85	109.67
1	N	2	VAL	N-CA-C	-5.06	101.12	109.12
1	N	37	GLN	CA-C-N	5.03	130.46	121.15
1	N	37	GLN	C-N-CA	5.03	130.46	121.15
1	N	37	GLN	N-CA-CB	5.03	118.57	110.42
1	N	203	HIS	CB-CA-C	-5.02	100.16	109.29
1	N	128	TYR	CA-CB-CG	-5.02	104.87	113.90
1	N	82	TYR	N-CA-C	5.01	119.40	113.28
1	N	179	GLY	CA-C-O	5.01	124.36	119.04
1	N	121	LEU	N-CA-CB	-5.01	102.60	109.97

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	108	TYR	Sidechain
1	N	123	ASN	Sidechain
1	N	128	TYR	Sidechain
1	N	136	ARG	Sidechain
1	N	149	TYR	Sidechain
1	N	159	SER	Peptide
1	N	163	TYR	Sidechain
1	N	168	VAL	Peptide
1	N	181	ARG	Sidechain
1	N	20	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	N	211	ARG	Sidechain
1	N	218	ARG	Sidechain
1	N	22	SER	Peptide
1	N	223	PHE	Sidechain
1	N	229	TYR	Sidechain
1	N	23	GLY	Peptide
1	N	239	SER	Peptide
1	N	36	ARG	Sidechain
1	N	48	ASP	Peptide
1	N	49	ARG	Sidechain
1	N	56	VAL	Mainchain
1	N	71	TYR	Sidechain
1	N	82	TYR	Sidechain
1	N	9	ARG	Sidechain
1	N	92	TYR	Sidechain
1	N	98	ARG	Sidechain

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	N	1822	0	1759	75	0
2	N	5	0	0	0	0
3	N	1	0	0	0	0
4	N	40	0	32	9	0
5	N	269	0	0	10	0
All	All	2137	0	1791	75	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 20.

All (75) 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:N:167:THR:HB	4:N:241:FR1:H372	1.32	1.10
1:N:167:THR:HB	4:N:241:FR1:C37	1.96	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:80:HIS:HD2	1:N:82:TYR:H	1.31	0.77
1:N:76:LYS:HB3	1:N:98:ARG:HB3	1.67	0.76
1:N:57:VAL:HG22	1:N:70:GLN:HG2	1.72	0.72
1:N:123:ASN:HD22	1:N:154:ASP:H	1.38	0.72
1:N:19:GLN:HG2	1:N:28:HIS:HA	1.71	0.71
1:N:48:ASP:N	1:N:49:ARG:HG2	2.06	0.71
1:N:153:VAL:HG23	1:N:157:ILE:HG13	1.73	0.71
1:N:48:ASP:CA	1:N:49:ARG:HG2	2.22	0.69
1:N:98:ARG:NH2	1:N:240:ASN:HB3	2.07	0.68
1:N:37:GLN:HB2	1:N:102:SER:HB3	1.77	0.67
1:N:170:ASN:HB3	5:N:1460:HOH:O	1.95	0.66
1:N:123:ASN:ND2	1:N:154:ASP:H	1.94	0.64
1:N:113:VAL:HG12	5:N:1476:HOH:O	1.97	0.64
1:N:57:VAL:CG2	1:N:70:GLN:HG2	2.26	0.64
1:N:80:HIS:CD2	1:N:82:TYR:H	2.15	0.64
1:N:191:PRO:HG3	5:N:1450:HOH:O	1.99	0.62
1:N:56:VAL:HG22	1:N:59:GLU:HB2	1.81	0.62
1:N:119:THR:O	1:N:120:ILE:HG13	2.00	0.62
1:N:191:PRO:HD3	5:N:1248:HOH:O	2.01	0.60
1:N:76:LYS:NZ	1:N:98:ARG:HH22	1.99	0.60
1:N:167:THR:HG21	4:N:241:FR1:O6	2.00	0.60
1:N:16:ILE:HD12	1:N:16:ILE:C	2.29	0.57
1:N:70:GLN:HE22	1:N:104:THR:H	1.51	0.56
1:N:167:THR:HB	4:N:241:FR1:H371	1.87	0.55
1:N:153:VAL:HG22	1:N:158:CYS:HB2	1.89	0.54
1:N:164:TRP:O	1:N:167:THR:HG23	2.07	0.54
1:N:63:ASN:O	1:N:64:GLN:C	2.45	0.54
1:N:36:ARG:HB2	1:N:39:TRP:HB2	1.90	0.54
1:N:229:TYR:HB2	5:N:1473:HOH:O	2.07	0.53
1:N:76:LYS:HZ3	1:N:98:ARG:HH22	1.56	0.53
1:N:15:GLN:NE2	5:N:1248:HOH:O	2.40	0.52
1:N:162:SER:OG	1:N:218:ARG:HD3	2.09	0.51
1:N:216:VAL:O	1:N:216:VAL:HG23	2.09	0.51
1:N:217:THR:HG22	1:N:218:ARG:HG3	1.92	0.51
1:N:209:VAL:O	4:N:241:FR1:H14	2.11	0.50
1:N:164:TRP:CB	1:N:168:VAL:HG23	2.42	0.50
1:N:63:ASN:O	1:N:64:GLN:O	2.29	0.49
1:N:19:GLN:HE22	1:N:54:ARG:HH11	1.61	0.49
1:N:119:THR:C	1:N:120:ILE:HG13	2.37	0.49
1:N:159:SER:O	1:N:160:SER:C	2.53	0.49
1:N:211:ARG:HA	4:N:241:FR1:C16	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:13:PRO:HB2	1:N:110:GLN:HB2	1.94	0.48
1:N:16:ILE:HG22	1:N:57:VAL:HG12	1.96	0.47
1:N:20:TYR:CE1	1:N:29:THR:HG23	2.48	0.47
1:N:185:GLN:NE2	1:N:185:GLN:H	2.13	0.47
1:N:101:GLN:HE21	1:N:102:SER:N	2.13	0.46
1:N:209:VAL:HG22	4:N:241:FR1:C29	2.46	0.46
1:N:185:GLN:NE2	1:N:214:CYS:SG	2.89	0.45
1:N:23:GLY:H	1:N:25:SER:H	1.64	0.44
1:N:84:ASN:OD1	1:N:86:ASP:N	2.49	0.44
1:N:48:ASP:C	1:N:49:ARG:HG2	2.34	0.44
1:N:129:ILE:HD13	1:N:129:ILE:HG21	1.65	0.44
1:N:38:ASN:HA	1:N:99:LEU:HD22	2.00	0.42
1:N:154:ASP:OD1	1:N:157:ILE:HG23	2.19	0.42
1:N:80:HIS:HD2	1:N:82:TYR:N	2.08	0.42
1:N:84:ASN:HA	5:N:1399:HOH:O	2.19	0.42
1:N:103:VAL:CG1	1:N:109:VAL:HG11	2.50	0.42
1:N:98:ARG:HH21	1:N:240:ASN:HB3	1.79	0.42
1:N:164:TRP:HH2	1:N:210:SER:HA	1.85	0.42
1:N:25:SER:HB2	1:N:26:TRP:H	1.45	0.41
1:N:45:HIS:CE1	4:N:241:FR1:H211	2.55	0.41
1:N:34:LEU:HD12	1:N:34:LEU:HA	1.76	0.41
1:N:216:VAL:HG21	1:N:219:LYS:HB2	2.01	0.41
1:N:37:GLN:HG3	5:N:1277:HOH:O	2.20	0.41
1:N:164:TRP:CE2	1:N:219:LYS:HB3	2.56	0.41
1:N:164:TRP:HZ3	4:N:241:FR1:HC2	1.85	0.41
1:N:226:VAL:HG13	5:N:1473:HOH:O	2.20	0.41
1:N:121:LEU:HD11	1:N:203:HIS:CE1	2.56	0.41
1:N:46:CYS:O	1:N:49:ARG:CZ	2.68	0.40
1:N:216:VAL:CG2	1:N:219:LYS:HB2	2.50	0.40
1:N:76:LYS:HG2	1:N:98:ARG:NH2	2.37	0.40
1:N:116:ARG:HD2	5:N:1412:HOH:O	2.21	0.40
1:N:169:LYS:HE2	1:N:169:LYS:HB3	1.63	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	N	238/240 (99%)	218 (92%)	17 (7%)	3 (1%)	9 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	64	GLN
1	N	160	SER
1	N	117	ALA

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	N	198/198 (100%)	154 (78%)	44 (22%)	1 1

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	6	GLU
1	N	8	GLN
1	N	11	SER
1	N	16	ILE
1	N	21	ARG
1	N	37	GLN
1	N	40	VAL
1	N	49	ARG
1	N	50	GLU
1	N	55	VAL
1	N	56	VAL
1	N	64	GLN
1	N	70	GLN
1	N	84	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	88	VAL
1	N	99	LEU
1	N	101	GLN
1	N	102	SER
1	N	103	VAL
1	N	104	THR
1	N	113	VAL
1	N	114	LEU
1	N	121	LEU
1	N	124	ASN
1	N	150	LEU
1	N	153	VAL
1	N	157	ILE
1	N	160	SER
1	N	161	SER
1	N	167	THR
1	N	168	VAL
1	N	170	ASN
1	N	181	ARG
1	N	185	GLN
1	N	195	LEU
1	N	196	VAL
1	N	205	VAL
1	N	210	SER
1	N	211	ARG
1	N	212	LEU
1	N	217	THR
1	N	222	VAL
1	N	230	ILE
1	N	240	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	15	GLN
1	N	19	GLN
1	N	70	GLN
1	N	80	HIS
1	N	101	GLN
1	N	123	ASN
1	N	170	ASN
1	N	185	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	199	GLN
1	N	234	ASN
1	N	240	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	SO4	N	1242	-	4,4,4	0.77	0	6,6,6	0.98	0
4	FR1	N	241	1	40,41,41	2.22	8 (20%)	55,59,59	3.07	18 (32%)

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
4	FR1	N	241	1	-	8/49/61/61	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	241	FR1	O32-C31	8.93	1.36	1.21
4	N	241	FR1	C33-C31	4.57	1.61	1.53
4	N	241	FR1	C4-N5	4.50	1.43	1.33
4	N	241	FR1	F34-C33	-3.23	1.18	1.32
4	N	241	FR1	C20-N19	3.14	1.53	1.47
4	N	241	FR1	C24-N26	-2.71	1.28	1.34
4	N	241	FR1	C37-C38	2.59	1.57	1.50
4	N	241	FR1	C10-N12	-2.55	1.28	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	241	FR1	O32-C31-C33	-18.08	103.31	117.06
4	N	241	FR1	C38-C37-N5	5.58	130.41	113.06
4	N	241	FR1	O11-C10-C9	4.26	129.34	120.90
4	N	241	FR1	C14-C13-C17	-3.31	104.23	110.71
4	N	241	FR1	C21-C20-C24	-3.09	104.65	111.21
4	N	241	FR1	C37-N5-C4	-3.01	114.04	121.29
4	N	241	FR1	C8-C7-C3	-2.87	117.73	120.80
4	N	241	FR1	C16-C14-C13	2.83	118.92	111.16
4	N	241	FR1	F35-C33-C31	2.67	118.08	112.14
4	N	241	FR1	F34-C33-C31	-2.65	106.22	112.14
4	N	241	FR1	C1-C2-C3	2.61	123.59	120.80
4	N	241	FR1	C9-C10-N12	-2.56	112.30	117.04
4	N	241	FR1	O39-C38-C37	-2.43	112.58	122.66
4	N	241	FR1	O40-C38-C37	2.43	122.03	112.81
4	N	241	FR1	C3-C4-N5	2.33	121.96	117.12
4	N	241	FR1	O11-C10-N12	-2.30	118.09	122.47
4	N	241	FR1	C23-N19-C20	2.17	115.42	112.01
4	N	241	FR1	C24-C20-N19	2.09	118.18	112.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	241	FR1	N26-C27-C31-O32
4	N	241	FR1	N12-C10-C9-C8
4	N	241	FR1	N12-C10-C9-C1
4	N	241	FR1	C28-C27-C31-O32
4	N	241	FR1	O11-C10-C9-C8
4	N	241	FR1	N5-C37-C38-O39

Continued on next page...

Continued from previous page...

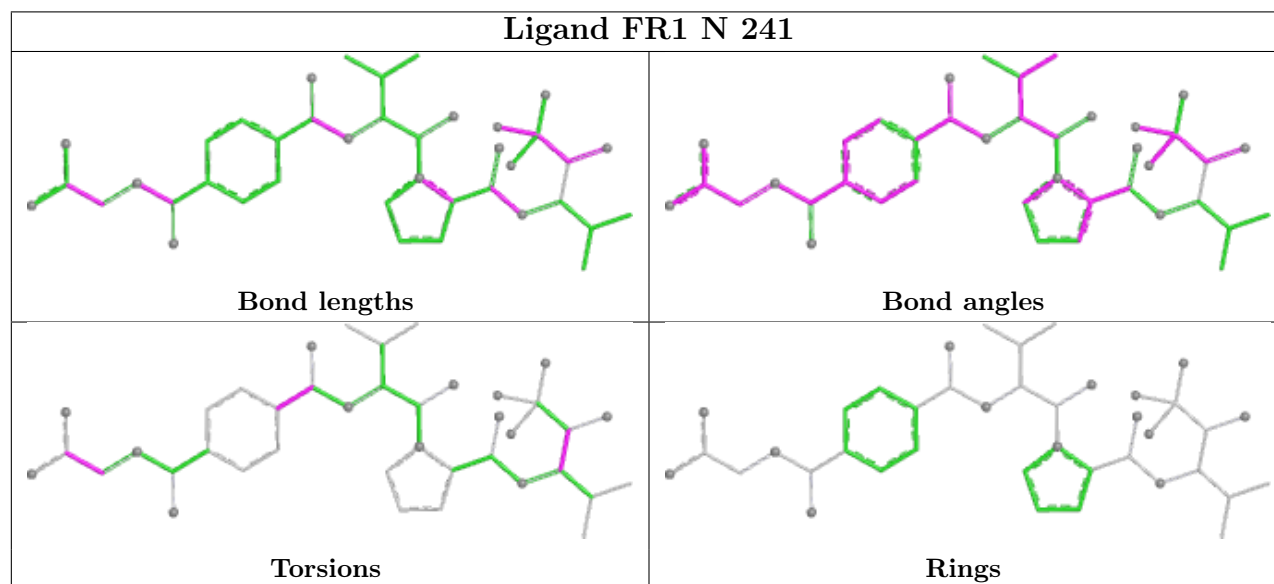
Mol	Chain	Res	Type	Atoms
4	N	241	FR1	N5-C37-C38-O40
4	N	241	FR1	O11-C10-C9-C1

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	241	FR1	9	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	N	240/240 (100%)	-0.15	0 100 100	6, 14, 22, 25	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

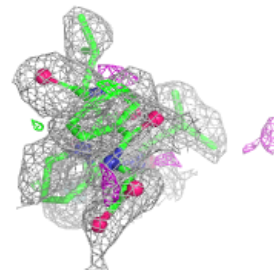
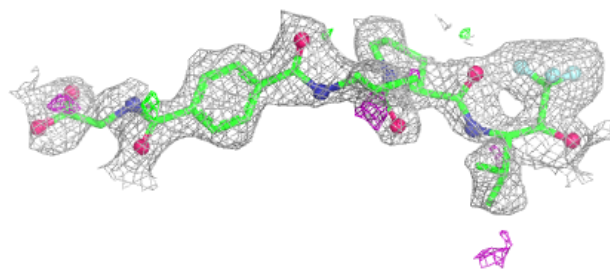
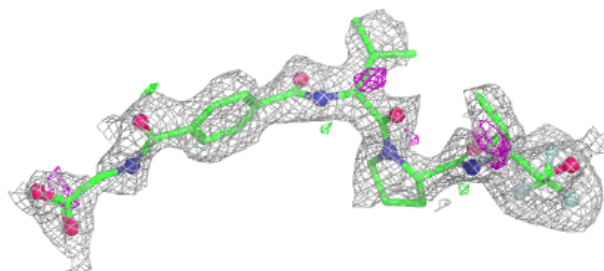
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FR1	N	241	40/40	0.89	0.10	14,22,29,30	0
3	CA	N	250	1/1	0.93	0.15	26,26,26,26	0
2	SO4	N	1242	5/5	0.97	0.08	19,20,22,22	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 FR1 N 241:

$2mF_o-DF_c$ (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.