Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 12:36 PM EDT

PDB ID	:	1MMJ
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 (i) 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 (i)) were used in the production of this report:

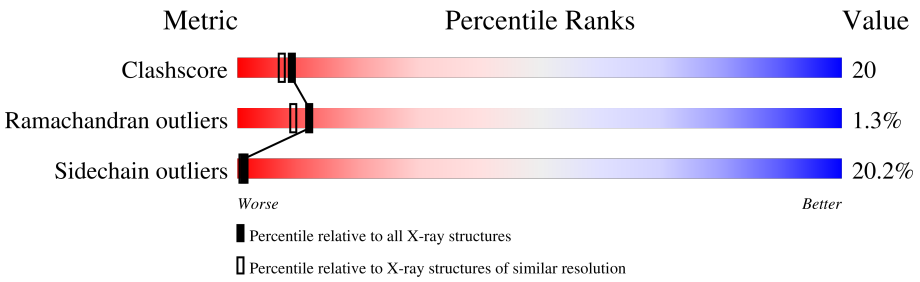
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 <=5%

Mol	Chain	Length	Quality of chain
1	N	240	40% 30% 20% 10%

2 Entry composition (i)

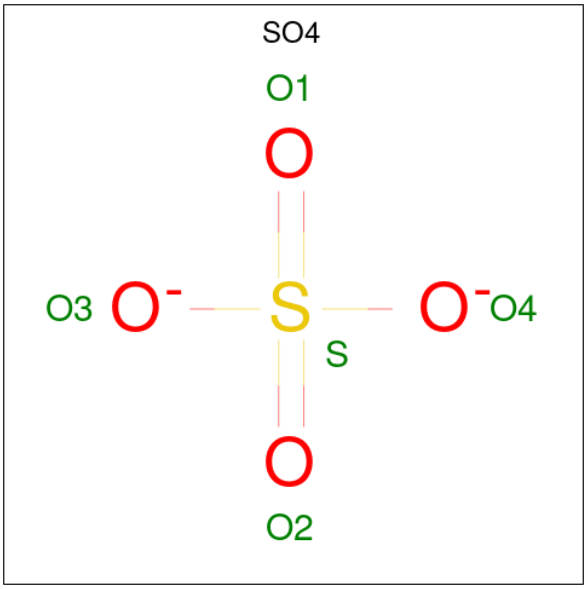
There are 5 unique types of molecules in this entry. The entry contains 2137 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: SO4) (formula: O_4S).



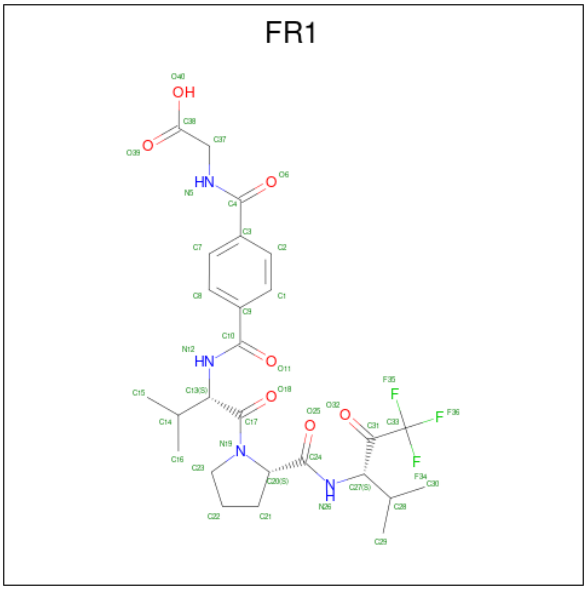
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	N	1	5	4	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: 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-OXOPRO

PYL]AMINOCARBONYL]PYRROLIDIN-1-YL-]CARBONYL]-2-METHYLPROPYL]AMINOCARBONYL]BENZOYLAMINO]ACETIC ACID (three-letter code: FR1) (formula: $C_{26}H_{33}F_3N_4O_7$).



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

- Molecule 5 is water.

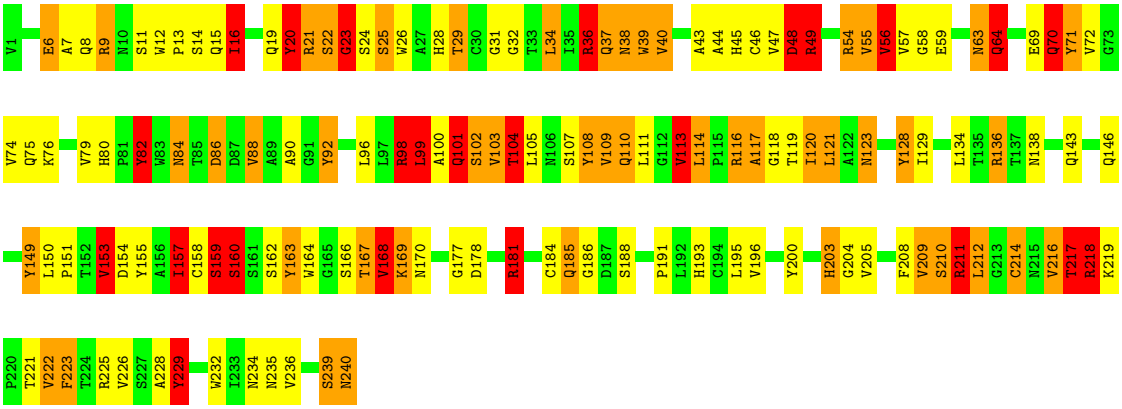
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	N	269	269	269	0	0

3 Residue-property plots (i)

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. 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. 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: 40% 30% 20% 10%



4 Data and refinement statistics (i)

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 42.43 – 1.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 77.1 (42.43-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.27 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA, FR1

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	1.93	33/1862 (1.8%)	2.67	146/2543 (5.7%)

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 (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	232	TRP	CD2-CE2	9.46	1.52	1.41
1	N	211	ARG	NE-CZ	7.88	1.43	1.33
1	N	177	GLY	CA-C	7.76	1.64	1.51
1	N	116	ARG	NE-CZ	7.00	1.42	1.33
1	N	204	GLY	N-CA	6.81	1.56	1.46
1	N	22	SER	CB-OG	6.59	1.50	1.42
1	N	98	ARG	NE-CZ	6.51	1.41	1.33
1	N	223	PHE	CG-CD2	6.32	1.48	1.38
1	N	90	ALA	C-N	6.11	1.44	1.33
1	N	31	GLY	N-CA	6.06	1.55	1.46
1	N	186	GLY	N-CA	6.04	1.55	1.46
1	N	138	ASN	C-N	5.96	1.43	1.33
1	N	181	ARG	NE-CZ	5.85	1.40	1.33
1	N	166	SER	CB-OG	5.81	1.49	1.42
1	N	214	CYS	CB-SG	5.79	1.92	1.82
1	N	58	GLY	N-CA	5.69	1.54	1.46
1	N	203	HIS	CG-CD2	5.67	1.45	1.35
1	N	159	SER	CA-CB	5.64	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	36	ARG	NE-CZ	5.53	1.40	1.33
1	N	39	TRP	CD2-CE2	5.53	1.48	1.41
1	N	31	GLY	CA-C	5.42	1.60	1.51
1	N	12	TRP	N-CA	5.39	1.57	1.46
1	N	193	HIS	CE1-NE2	5.38	1.45	1.32
1	N	32	GLY	CA-C	5.38	1.60	1.51
1	N	101	GLN	CB-CG	5.32	1.67	1.52
1	N	203	HIS	CE1-NE2	5.29	1.44	1.32
1	N	7	ALA	CA-CB	5.25	1.63	1.52
1	N	21	ARG	NE-CZ	5.25	1.39	1.33
1	N	177	GLY	N-CA	5.20	1.53	1.46
1	N	146	GLN	CG-CD	5.20	1.63	1.51
1	N	208	PHE	CG-CD2	5.04	1.46	1.38
1	N	163	TYR	CE2-CZ	5.03	1.45	1.38
1	N	235	ASN	N-CA	5.00	1.56	1.46

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	116	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	N	181	ARG	NE-CZ-NH2	14.96	127.78	120.30
1	N	136	ARG	NE-CZ-NH1	-12.03	114.29	120.30
1	N	104	THR	CA-CB-CG2	-11.89	95.75	112.40
1	N	114	LEU	CB-CG-CD2	11.40	130.38	111.00
1	N	64	GLN	CA-CB-CG	11.19	138.01	113.40
1	N	228	ALA	CB-CA-C	-10.84	93.84	110.10
1	N	21	ARG	NE-CZ-NH2	-10.59	115.00	120.30
1	N	36	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	N	163	TYR	CB-CG-CD1	-10.37	114.78	121.00
1	N	22	SER	N-CA-CB	10.36	126.04	110.50
1	N	79	VAL	CG1-CB-CG2	-10.26	94.49	110.90
1	N	72	VAL	CG1-CB-CG2	-10.18	94.61	110.90
1	N	212	LEU	CB-CA-C	-10.16	90.89	110.20
1	N	218	ARG	CD-NE-CZ	-9.87	109.78	123.60
1	N	14	SER	N-CA-CB	9.78	125.17	110.50
1	N	181	ARG	CA-CB-CG	9.62	134.57	113.40
1	N	36	ARG	CD-NE-CZ	-9.41	110.43	123.60
1	N	22	SER	CB-CA-C	-9.38	92.28	110.10
1	N	209	VAL	CG1-CB-CG2	9.35	125.86	110.90
1	N	181	ARG	NH1-CZ-NH2	-9.32	109.15	119.40
1	N	222	VAL	CA-CB-CG2	9.29	124.83	110.90
1	N	103	VAL	N-CA-CB	-9.16	91.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	108	TYR	CB-CG-CD1	-9.12	115.53	121.00
1	N	120	ILE	CA-CB-CG1	-9.05	93.81	111.00
1	N	225	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	N	149	TYR	CB-CG-CD1	-8.93	115.64	121.00
1	N	44	ALA	CB-CA-C	-8.86	96.80	110.10
1	N	181	ARG	CD-NE-CZ	-8.69	111.43	123.60
1	N	29	THR	CA-CB-CG2	8.68	124.55	112.40
1	N	128	TYR	CB-CG-CD1	-8.66	115.80	121.00
1	N	229	TYR	CB-CG-CD2	-8.60	115.84	121.00
1	N	116	ARG	CB-CG-CD	8.49	133.68	111.60
1	N	100	ALA	N-CA-CB	-8.30	98.48	110.10
1	N	71	TYR	CB-CG-CD2	-8.20	116.08	121.00
1	N	223	PHE	CZ-CE2-CD2	-8.12	110.36	120.10
1	N	109	VAL	CG1-CB-CG2	8.10	123.87	110.90
1	N	38	ASN	CB-CG-OD1	8.07	137.74	121.60
1	N	218	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	N	24	SER	N-CA-C	8.01	132.62	111.00
1	N	82	TYR	CZ-CE2-CD2	-7.83	112.75	119.80
1	N	20	TYR	CA-C-N	-7.82	99.99	117.20
1	N	36	ARG	NH1-CZ-NH2	-7.81	110.81	119.40
1	N	47	VAL	CA-CB-CG1	-7.67	99.39	110.90
1	N	134	LEU	CB-CG-CD2	-7.63	98.02	111.00
1	N	116	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	N	225	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	N	103	VAL	CA-CB-CG1	7.15	121.62	110.90
1	N	56	VAL	CA-CB-CG2	7.10	121.55	110.90
1	N	116	ARG	CD-NE-CZ	7.03	133.44	123.60
1	N	6	GLU	CB-CA-C	7.01	124.42	110.40
1	N	14	SER	CB-CA-C	-7.00	96.80	110.10
1	N	229	TYR	CG-CD2-CE2	-6.98	115.72	121.30
1	N	55	VAL	CA-CB-CG1	6.92	121.29	110.90
1	N	203	HIS	C-N-CA	-6.90	107.80	122.30
1	N	113	VAL	CG1-CB-CG2	-6.83	99.97	110.90
1	N	168	VAL	CA-CB-CG1	6.79	121.08	110.90
1	N	216	VAL	CG1-CB-CG2	6.63	121.51	110.90
1	N	153	VAL	CA-CB-CG1	6.61	120.81	110.90
1	N	40	VAL	CA-CB-CG2	6.55	120.72	110.90
1	N	166	SER	CB-CA-C	-6.50	97.75	110.10
1	N	20	TYR	CA-C-O	6.46	133.68	120.10
1	N	111	LEU	CB-CG-CD1	-6.46	100.02	111.00
1	N	9	ARG	CB-CA-C	-6.46	97.48	110.40
1	N	105	LEU	O-C-N	6.38	132.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	99	LEU	CB-CA-C	-6.35	98.14	110.20
1	N	149	TYR	CG-CD2-CE2	-6.27	116.29	121.30
1	N	166	SER	C-N-CA	-6.25	106.07	121.70
1	N	222	VAL	CA-CB-CG1	6.25	120.27	110.90
1	N	128	TYR	CD1-CE1-CZ	-6.23	114.19	119.80
1	N	212	LEU	N-CA-CB	6.19	122.78	110.40
1	N	234	ASN	N-CA-CB	-6.18	99.48	110.60
1	N	70	GLN	CA-CB-CG	6.07	126.75	113.40
1	N	143	GLN	CB-CG-CD	-6.05	95.87	111.60
1	N	149	TYR	CD1-CE1-CZ	-6.03	114.37	119.80
1	N	188	SER	CB-CA-C	-6.03	98.64	110.10
1	N	143	GLN	CA-CB-CG	5.99	126.59	113.40
1	N	108	TYR	N-CA-CB	-5.97	99.85	110.60
1	N	110	GLN	CG-CD-NE2	-5.96	102.40	116.70
1	N	101	GLN	CG-CD-OE1	5.91	133.43	121.60
1	N	149	TYR	CD1-CG-CD2	5.89	124.38	117.90
1	N	200	TYR	CB-CG-CD1	5.84	124.50	121.00
1	N	221	THR	C-N-CA	-5.84	107.11	121.70
1	N	49	ARG	N-CA-CB	-5.83	100.11	110.60
1	N	232	TRP	CG-CD1-NE1	5.80	115.90	110.10
1	N	98	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	N	217	THR	CB-CA-C	-5.79	95.96	111.60
1	N	40	VAL	CG1-CB-CG2	5.78	120.14	110.90
1	N	101	GLN	CA-CB-CG	5.76	126.07	113.40
1	N	128	TYR	CD1-CG-CD2	5.75	124.23	117.90
1	N	169	LYS	N-CA-C	5.74	126.50	111.00
1	N	56	VAL	CG1-CB-CG2	5.73	120.07	110.90
1	N	34	LEU	CD1-CG-CD2	-5.71	93.36	110.50
1	N	48	ASP	CA-CB-CG	-5.70	100.87	113.40
1	N	153	VAL	CA-CB-CG2	5.69	119.43	110.90
1	N	178	ASP	N-CA-C	5.67	126.31	111.00
1	N	107	SER	N-CA-CB	5.60	118.89	110.50
1	N	163	TYR	C-N-CA	-5.58	107.75	121.70
1	N	29	THR	CB-CA-C	-5.57	96.56	111.60
1	N	54	ARG	CG-CD-NE	-5.56	100.11	111.80
1	N	239	SER	CB-CA-C	-5.56	99.54	110.10
1	N	98	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	N	118	GLY	N-CA-C	5.50	126.84	113.10
1	N	54	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	N	6	GLU	CA-CB-CG	5.47	125.43	113.40
1	N	49	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	N	229	TYR	CD1-CG-CD2	5.46	123.90	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	96	LEU	CA-C-O	5.45	131.54	120.10
1	N	25	SER	CB-CA-C	-5.45	99.75	110.10
1	N	71	TYR	CZ-CE2-CD2	-5.41	114.94	119.80
1	N	88	VAL	CG1-CB-CG2	5.39	119.52	110.90
1	N	25	SER	N-CA-CB	5.38	118.57	110.50
1	N	23	GLY	CA-C-N	-5.35	105.42	117.20
1	N	200	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	N	108	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
1	N	92	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	N	63	ASN	CB-CG-OD1	5.30	132.20	121.60
1	N	236	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	N	38	ASN	CB-CG-ND2	-5.28	104.03	116.70
1	N	39	TRP	CD2-CE3-CZ3	-5.27	111.95	118.80
1	N	128	TYR	CG-CD2-CE2	-5.25	117.10	121.30
1	N	157	ILE	CA-CB-CG2	5.23	121.36	110.90
1	N	98	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
1	N	223	PHE	CE1-CZ-CE2	5.20	129.35	120.00
1	N	159	SER	N-CA-C	5.18	124.98	111.00
1	N	70	GLN	N-CA-CB	5.18	119.92	110.60
1	N	63	ASN	C-N-CA	-5.17	108.78	121.70
1	N	69	GLU	CA-CB-CG	5.16	124.76	113.40
1	N	117	ALA	C-N-CA	-5.16	111.46	122.30
1	N	92	TYR	C-N-CA	-5.15	108.82	121.70
1	N	134	LEU	CD1-CG-CD2	5.14	125.93	110.50
1	N	16	ILE	CA-CB-CG1	5.13	120.74	111.00
1	N	203	HIS	CB-CA-C	-5.12	100.16	110.40
1	N	193	HIS	CB-CA-C	-5.10	100.20	110.40
1	N	117	ALA	N-CA-CB	-5.10	102.97	110.10
1	N	159	SER	CA-CB-OG	5.08	124.93	111.20
1	N	108	TYR	CG-CD2-CE2	-5.08	117.24	121.30
1	N	151	PRO	CA-C-N	-5.08	106.03	117.20
1	N	43	ALA	CB-CA-C	-5.07	102.49	110.10
1	N	24	SER	C-N-CA	-5.07	109.02	121.70
1	N	24	SER	CB-CA-C	-5.06	100.48	110.10
1	N	49	ARG	CG-CD-NE	-5.06	101.17	111.80
1	N	155	TYR	CB-CA-C	-5.05	100.30	110.40
1	N	74	VAL	CA-CB-CG1	5.04	118.46	110.90
1	N	56	VAL	CA-C-N	-5.02	106.15	117.20
1	N	86	ASP	N-CA-C	5.02	124.55	111.00

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
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1822	0	1759	74	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	74	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 (74) 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
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:76:LYS:HZ3	1:N:98:ARG:HH22	1.49	0.58
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:36:ARG:HB2	1:N:39:TRP:HB2	1.90	0.54
1:N:16:ILE:HD12	1:N:16:ILE:C	2.29	0.53
1:N:229:TYR:HB2	5:N:1473:HOH:O	2.07	0.53
1:N:15:GLN:NE2	5:N:1248:HOH:O	2.40	0.52
1:N:63:ASN:O	1:N:64:GLN:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:ARG:HA	4:N:241:FR1:C16	2.42	0.49
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:159:SER:O	1:N:160:SER:C	2.53	0.45
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:119:THR:C	1:N:120:ILE:HG13	2.37	0.44
1:N:84:ASN:OD1	1:N:86:ASP:N	2.49	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	238/240 (99%)	218 (92%)	17 (7%)	3 (1%)	12 9

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	198/198 (100%)	158 (80%)	40 (20%)	1 1

All (40) 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	48	ASP

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Mol	Chain	Res	Type
1	N	49	ARG
1	N	55	VAL
1	N	56	VAL
1	N	64	GLN
1	N	70	GLN
1	N	75	GLN
1	N	84	ASN
1	N	88	VAL
1	N	99	LEU
1	N	101	GLN
1	N	102	SER
1	N	104	THR
1	N	113	VAL
1	N	114	LEU
1	N	121	LEU
1	N	150	LEU
1	N	153	VAL
1	N	157	ILE
1	N	160	SER
1	N	167	THR
1	N	181	ARG
1	N	184	CYS
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	240	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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

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Mol	Chain	Res	Type
1	N	124	ASN
1	N	185	GLN
1	N	199	GLN
1	N	234	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 monosaccharides 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	$\#\|Z\| > 2$
4	FR1	N	241	1	40,41,41	2.16	8 (20%)	55,59,59	3.07	19 (34%)
2	SO4	N	1242	-	4,4,4	0.72	0	6,6,6	1.03	0

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	8.46	1.36	1.21
4	N	241	FR1	C33-C31	4.57	1.61	1.53
4	N	241	FR1	C4-N5	4.51	1.43	1.33
4	N	241	FR1	F34-C33	-3.04	1.18	1.32
4	N	241	FR1	C20-N19	3.03	1.53	1.47
4	N	241	FR1	C37-C38	2.88	1.57	1.51
4	N	241	FR1	C10-N12	-2.68	1.28	1.34
4	N	241	FR1	C24-N26	-2.63	1.28	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	241	FR1	O32-C31-C33	-18.08	103.31	117.06
4	N	241	FR1	C38-C37-N5	5.63	130.41	113.06
4	N	241	FR1	O11-C10-C9	4.71	129.34	120.94
4	N	241	FR1	C14-C13-C17	-3.21	104.23	110.73
4	N	241	FR1	C21-C20-C24	-3.08	104.65	111.22
4	N	241	FR1	C37-N5-C4	-3.06	114.04	121.33
4	N	241	FR1	C16-C14-C13	2.75	118.92	111.16
4	N	241	FR1	O40-C38-C37	2.67	122.03	112.74
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	C8-C7-C3	-2.62	117.73	120.78
4	N	241	FR1	O39-C38-C37	-2.50	112.58	122.68
4	N	241	FR1	C9-C10-N12	-2.48	112.30	117.06
4	N	241	FR1	C1-C2-C3	2.41	123.59	120.78
4	N	241	FR1	O11-C10-N12	-2.37	118.09	122.45
4	N	241	FR1	C3-C4-N5	2.27	121.96	117.09
4	N	241	FR1	C23-N19-C20	2.16	115.42	112.00
4	N	241	FR1	C13-N12-C10	-2.14	117.65	121.52
4	N	241	FR1	C24-C20-N19	2.04	118.18	112.56

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

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Mol	Chain	Res	Type	Atoms
4	N	241	FR1	N12-C10-C9-C8
4	N	241	FR1	N12-C10-C9-C1
4	N	241	FR1	O11-C10-C9-C8
4	N	241	FR1	N5-C37-C38-O39
4	N	241	FR1	N5-C37-C38-O40
4	N	241	FR1	O11-C10-C9-C1
4	N	241	FR1	C28-C27-C31-O32

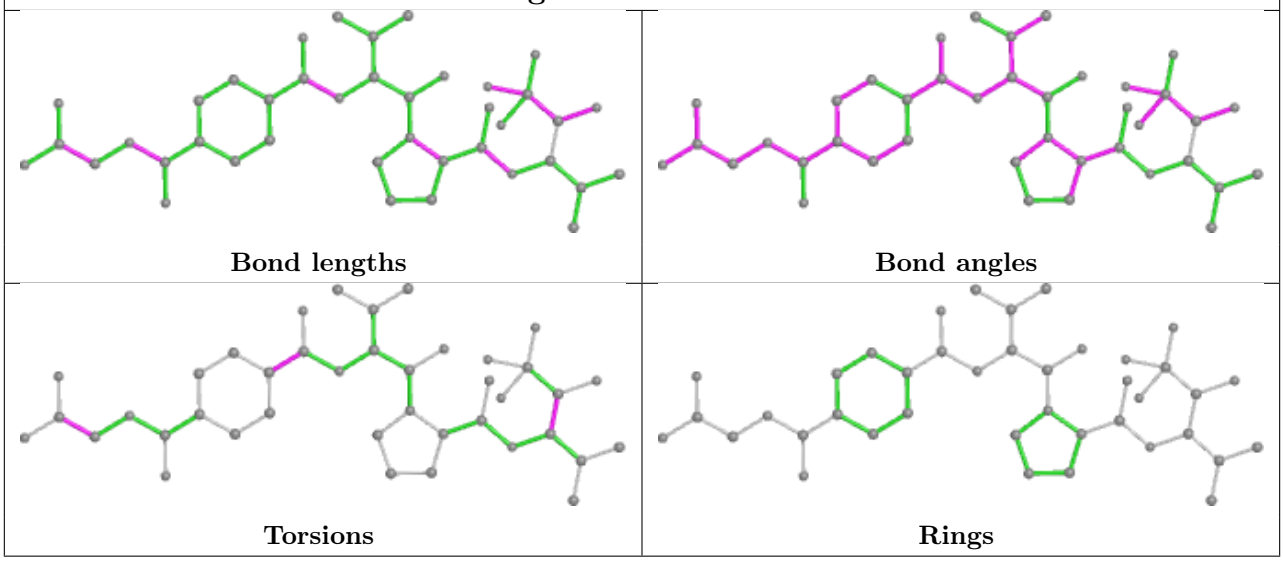
There are no ring outliers.

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 then 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.

Ligand FR1 N 241



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

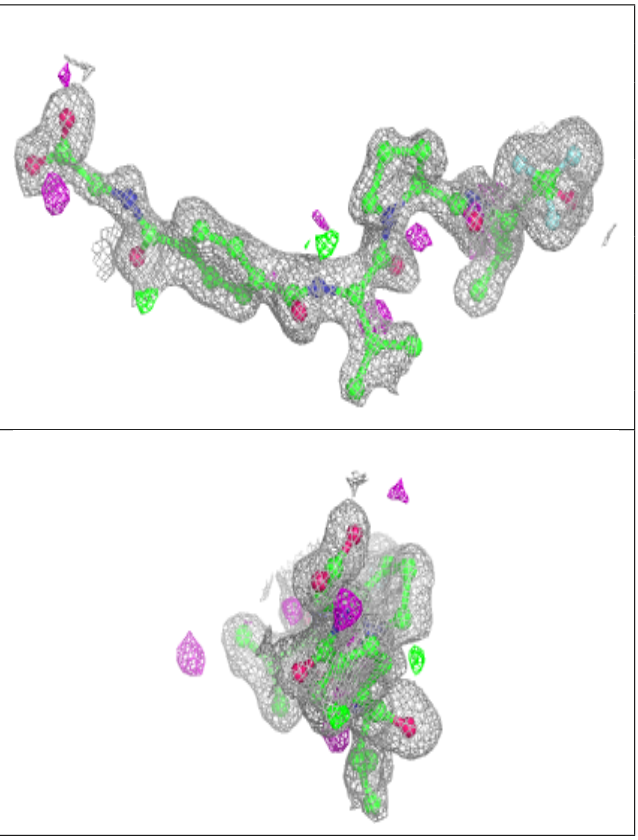
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.