



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:50 PM UTC

PDB ID : 4OMC / pdb_00004omc
Title : X-ray structure of human furin in complex with the competitive inhibitor meta-guanidinomethyl-Phac-RVR-Amba
Authors : Dahms, S.O.; Than, M.E.
Deposited on : 2014-01-27
Resolution : 2.30 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
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

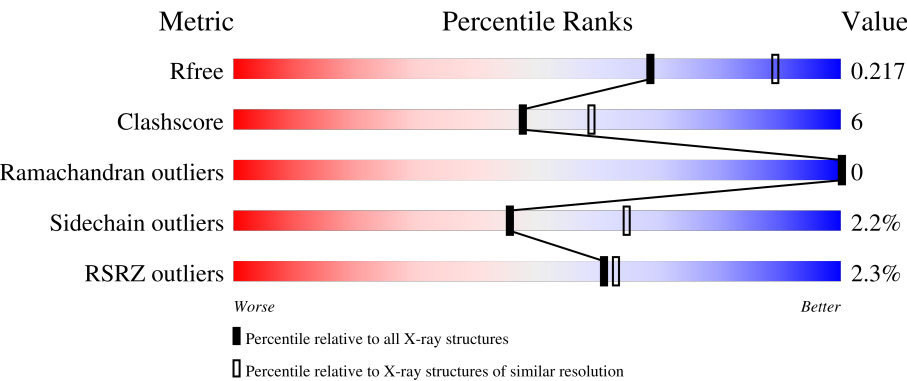
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	482	2% 82% 14% ..
1	B	482	2% 82% 13% ..
1	C	482	2% 82% 14% ..
1	D	482	2% 83% 12% ..
1	E	482	2% 82% 13% ..

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Mol	Chain	Length	Quality of chain
1	F	482	2% 79% 16% ...
2	H	5	100%
2	I	5	100%
2	J	5	100%
2	K	5	100%
2	L	5	100%
2	N	5	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23092 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 Furin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	34	0	0
			3559	2204	637	704	14			
1	B	465	Total	C	N	O	S	41	0	0
			3552	2199	636	703	14			
1	C	466	Total	C	N	O	S	36	0	0
			3559	2204	637	704	14			
1	D	465	Total	C	N	O	S	46	0	0
			3552	2199	636	703	14			
1	E	465	Total	C	N	O	S	40	0	0
			3552	2199	636	703	14			
1	F	465	Total	C	N	O	S	56	0	0
			3552	2199	636	703	14			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	expression tag	UNP P09958
A	576	GLY	-	expression tag	UNP P09958
A	577	SER	-	expression tag	UNP P09958
A	578	LEU	-	expression tag	UNP P09958
A	579	VAL	-	expression tag	UNP P09958
A	580	PRO	-	expression tag	UNP P09958
A	581	ARG	-	expression tag	UNP P09958
A	582	GLY	-	expression tag	UNP P09958
A	583	SER	-	expression tag	UNP P09958
A	584	HIS	-	expression tag	UNP P09958
A	585	HIS	-	expression tag	UNP P09958
A	586	HIS	-	expression tag	UNP P09958
A	587	HIS	-	expression tag	UNP P09958
A	588	HIS	-	expression tag	UNP P09958
A	589	HIS	-	expression tag	UNP P09958
B	575	SER	-	expression tag	UNP P09958
B	576	GLY	-	expression tag	UNP P09958

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Chain	Residue	Modelled	Actual	Comment	Reference
B	577	SER	-	expression tag	UNP P09958
B	578	LEU	-	expression tag	UNP P09958
B	579	VAL	-	expression tag	UNP P09958
B	580	PRO	-	expression tag	UNP P09958
B	581	ARG	-	expression tag	UNP P09958
B	582	GLY	-	expression tag	UNP P09958
B	583	SER	-	expression tag	UNP P09958
B	584	HIS	-	expression tag	UNP P09958
B	585	HIS	-	expression tag	UNP P09958
B	586	HIS	-	expression tag	UNP P09958
B	587	HIS	-	expression tag	UNP P09958
B	588	HIS	-	expression tag	UNP P09958
B	589	HIS	-	expression tag	UNP P09958
C	575	SER	-	expression tag	UNP P09958
C	576	GLY	-	expression tag	UNP P09958
C	577	SER	-	expression tag	UNP P09958
C	578	LEU	-	expression tag	UNP P09958
C	579	VAL	-	expression tag	UNP P09958
C	580	PRO	-	expression tag	UNP P09958
C	581	ARG	-	expression tag	UNP P09958
C	582	GLY	-	expression tag	UNP P09958
C	583	SER	-	expression tag	UNP P09958
C	584	HIS	-	expression tag	UNP P09958
C	585	HIS	-	expression tag	UNP P09958
C	586	HIS	-	expression tag	UNP P09958
C	587	HIS	-	expression tag	UNP P09958
C	588	HIS	-	expression tag	UNP P09958
C	589	HIS	-	expression tag	UNP P09958
D	575	SER	-	expression tag	UNP P09958
D	576	GLY	-	expression tag	UNP P09958
D	577	SER	-	expression tag	UNP P09958
D	578	LEU	-	expression tag	UNP P09958
D	579	VAL	-	expression tag	UNP P09958
D	580	PRO	-	expression tag	UNP P09958
D	581	ARG	-	expression tag	UNP P09958
D	582	GLY	-	expression tag	UNP P09958
D	583	SER	-	expression tag	UNP P09958
D	584	HIS	-	expression tag	UNP P09958
D	585	HIS	-	expression tag	UNP P09958
D	586	HIS	-	expression tag	UNP P09958
D	587	HIS	-	expression tag	UNP P09958
D	588	HIS	-	expression tag	UNP P09958

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Chain	Residue	Modelled	Actual	Comment	Reference
D	589	HIS	-	expression tag	UNP P09958
E	575	SER	-	expression tag	UNP P09958
E	576	GLY	-	expression tag	UNP P09958
E	577	SER	-	expression tag	UNP P09958
E	578	LEU	-	expression tag	UNP P09958
E	579	VAL	-	expression tag	UNP P09958
E	580	PRO	-	expression tag	UNP P09958
E	581	ARG	-	expression tag	UNP P09958
E	582	GLY	-	expression tag	UNP P09958
E	583	SER	-	expression tag	UNP P09958
E	584	HIS	-	expression tag	UNP P09958
E	585	HIS	-	expression tag	UNP P09958
E	586	HIS	-	expression tag	UNP P09958
E	587	HIS	-	expression tag	UNP P09958
E	588	HIS	-	expression tag	UNP P09958
E	589	HIS	-	expression tag	UNP P09958
F	575	SER	-	expression tag	UNP P09958
F	576	GLY	-	expression tag	UNP P09958
F	577	SER	-	expression tag	UNP P09958
F	578	LEU	-	expression tag	UNP P09958
F	579	VAL	-	expression tag	UNP P09958
F	580	PRO	-	expression tag	UNP P09958
F	581	ARG	-	expression tag	UNP P09958
F	582	GLY	-	expression tag	UNP P09958
F	583	SER	-	expression tag	UNP P09958
F	584	HIS	-	expression tag	UNP P09958
F	585	HIS	-	expression tag	UNP P09958
F	586	HIS	-	expression tag	UNP P09958
F	587	HIS	-	expression tag	UNP P09958
F	588	HIS	-	expression tag	UNP P09958
F	589	HIS	-	expression tag	UNP P09958

- Molecule 2 is a protein called meta-guanidinomethyl-phenylacetyl-Arg-Val-Arg-(amidomethyl)benzamidine.

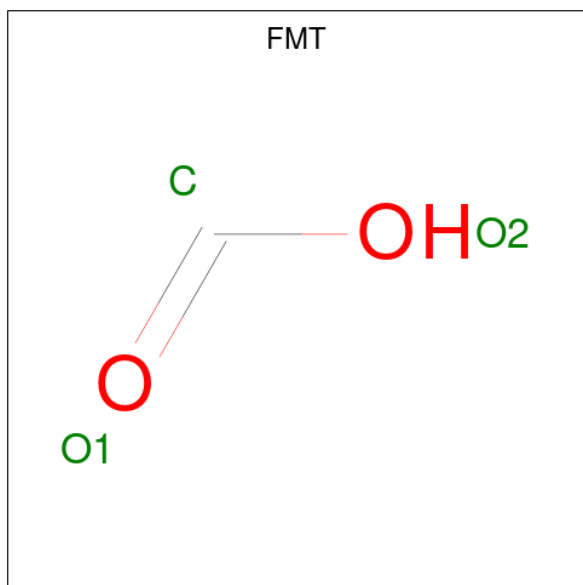
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	5	Total	C	N	O	0	0	0
			54	35	15	4			
2	I	5	Total	C	N	O	0	0	0
			54	35	15	4			
2	J	5	Total	C	N	O	0	0	0
			54	35	15	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	5	Total	C	N	O	0	0	0
			54	35	15	4			
2	L	5	Total	C	N	O	0	0	0
			54	35	15	4			
2	N	5	Total	C	N	O	0	0	0
			54	35	15	4			

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Ca 3 3	0	0
4	B	3	Total Ca 3 3	0	0
4	C	3	Total Ca 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	Ca 3	0	0
4	E	3	Total 3	Ca 3	0	0
4	F	3	Total 3	Ca 3	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Na 1	0	0
5	B	1	Total 1	Na 1	0	0
5	C	1	Total 1	Na 1	0	0
5	D	1	Total 1	Na 1	0	0
5	E	1	Total 1	Na 1	0	0
5	F	1	Total 1	Na 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	244	Total 244	O 244	0	0
6	B	216	Total 216	O 216	0	0
6	C	236	Total 236	O 236	0	0
6	D	218	Total 218	O 218	0	0
6	E	209	Total 209	O 209	0	0
6	F	193	Total 193	O 193	0	0
6	H	5	Total 5	O 5	0	0
6	I	5	Total 5	O 5	0	0

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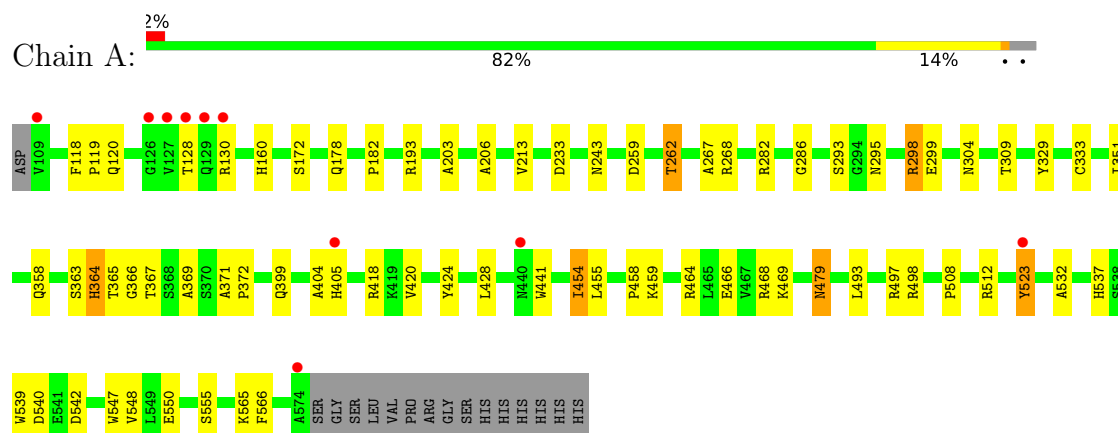
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	6	Total 6	O 6	0	0
6	K	5	Total 5	O 5	0	0
6	L	3	Total 3	O 3	0	0
6	N	6	Total 6	O 6	0	0

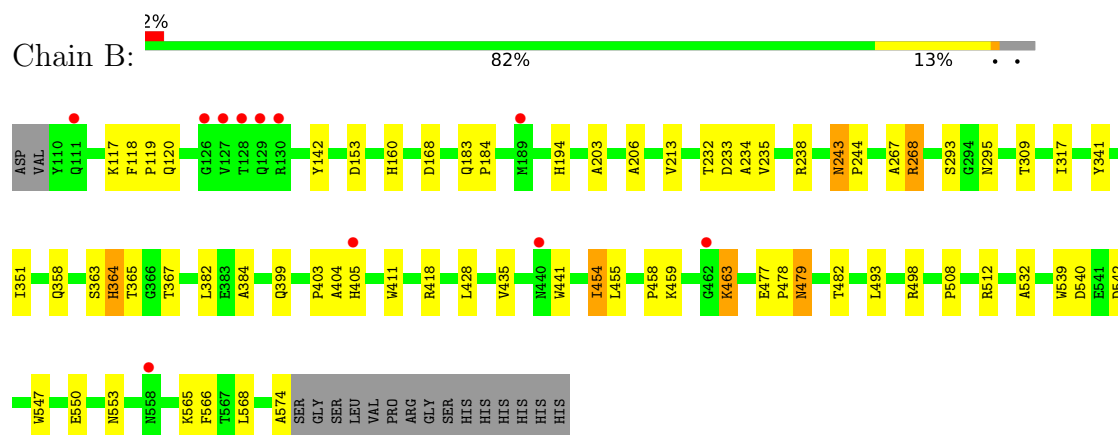
3 Residue-property plots [i](#)

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 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.

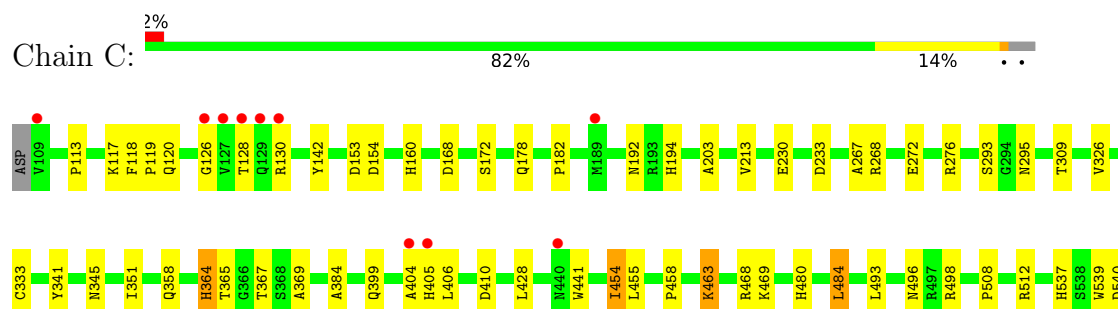
• Molecule 1: Furin



• Molecule 1: Furin

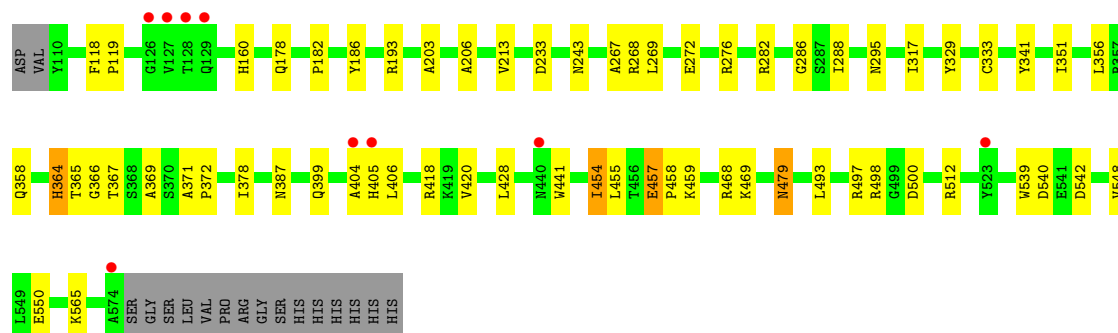
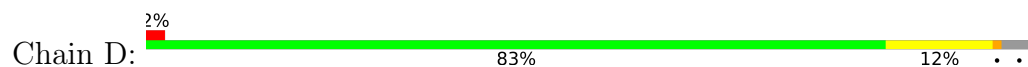


• Molecule 1: Furin

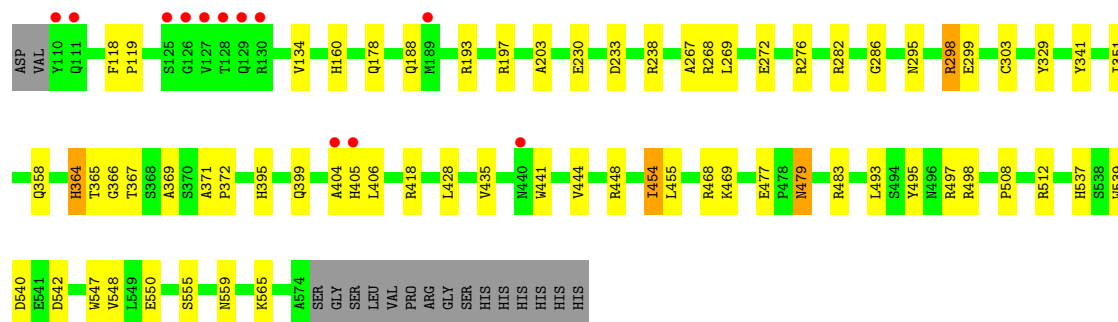
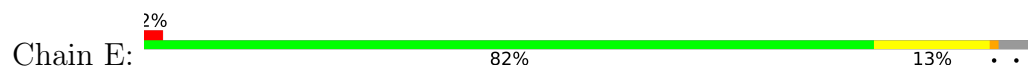




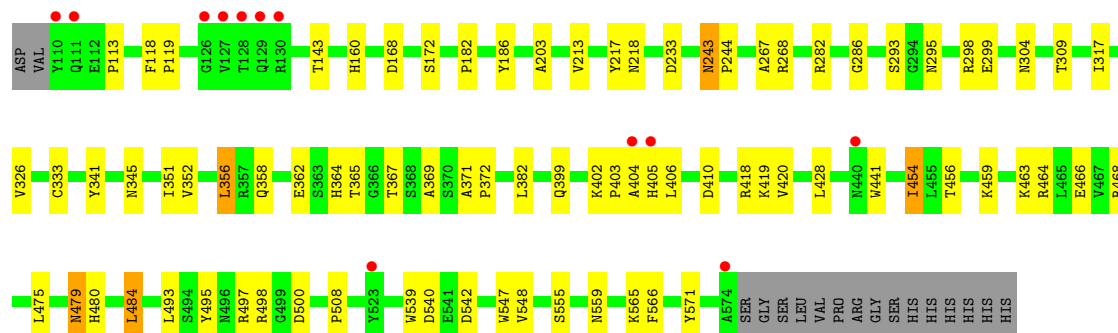
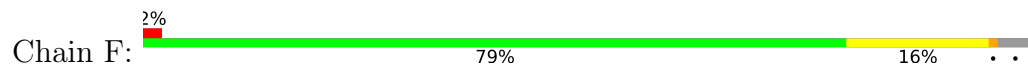
• Molecule 1: Furin



• Molecule 1: Furin



• Molecule 1: Furin



• Molecule 2: meta-guanidinomethyl-phenylacetyl-Arg-Val-Arg-(amidomethyl)benzamidine



There are no outlier residues recorded for this chain.

- Molecule 2: meta-guanidinomethyl-phenylacetyl-Arg-Val-Arg-(amidomethyl)benzamidine

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: meta-guanidinomethyl-phenylacetyl-Arg-Val-Arg-(amidomethyl)benzamidine

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: meta-guanidinomethyl-phenylacetyl-Arg-Val-Arg-(amidomethyl)benzamidine

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: meta-guanidinomethyl-phenylacetyl-Arg-Val-Arg-(amidomethyl)benzamidine

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: meta-guanidinomethyl-phenylacetyl-Arg-Val-Arg-(amidomethyl)benzamidine

Chain N:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.18Å 152.85Å 168.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.30) 99.5 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.185 , 0.216 0.185 , 0.217	Depositor DCC
R_{free} test set	8055 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23092	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: 00S, FMT, CA, NA, 2UC

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	0/3641	0.97	14/4964 (0.3%)
1	B	0.46	0/3634	0.97	13/4954 (0.3%)
1	C	0.48	0/3641	0.97	14/4964 (0.3%)
1	D	0.47	0/3634	0.96	12/4954 (0.2%)
1	E	0.46	0/3634	0.96	11/4954 (0.2%)
1	F	0.46	0/3634	0.96	13/4954 (0.3%)
2	H	0.33	0/28	0.99	0/35
2	I	0.28	0/28	1.03	0/35
2	J	0.34	0/28	1.02	0/35
2	K	0.26	0/28	1.01	0/35
2	L	0.35	0/28	1.01	0/35
2	N	0.31	0/28	1.07	0/35
All	All	0.47	0/21986	0.97	77/29954 (0.3%)

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	A	0	1

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	454	ILE	N-CA-C	9.68	121.84	111.58
1	C	454	ILE	N-CA-C	9.60	120.37	111.45
1	D	454	ILE	N-CA-C	9.58	120.36	111.45
1	A	454	ILE	N-CA-C	9.42	120.21	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	454	ILE	N-CA-C	9.24	120.04	111.45
1	B	454	ILE	N-CA-C	9.18	121.31	111.58
1	A	268	ARG	N-CA-C	8.32	121.10	111.11
1	B	268	ARG	N-CA-C	8.16	120.90	111.11
1	F	268	ARG	N-CA-C	7.96	120.66	111.11
1	C	268	ARG	N-CA-C	7.88	120.57	111.11
1	E	268	ARG	N-CA-C	7.59	120.22	111.11
1	A	203	ALA	N-CA-C	7.54	120.04	110.61
1	B	203	ALA	N-CA-C	7.45	119.93	110.61
1	F	203	ALA	N-CA-C	7.42	119.88	110.61
1	D	268	ARG	N-CA-C	7.41	120.00	111.11
1	D	203	ALA	N-CA-C	7.32	119.76	110.61
1	C	203	ALA	N-CA-C	7.06	119.44	110.61
1	A	365	THR	N-CA-C	6.97	118.68	108.86
1	E	203	ALA	N-CA-C	6.97	119.32	110.61
1	F	365	THR	N-CA-C	6.93	119.03	109.18
1	B	542	ASP	N-CA-C	-6.79	99.80	109.24
1	D	365	THR	N-CA-C	6.71	118.71	109.18
1	C	542	ASP	N-CA-C	-6.69	99.95	109.24
1	F	243	ASN	CB-CA-C	-6.64	106.49	111.20
1	E	542	ASP	N-CA-C	-6.62	100.04	109.24
1	C	365	THR	N-CA-C	6.57	118.13	108.86
1	D	542	ASP	N-CA-C	-6.51	100.19	109.24
1	E	365	THR	N-CA-C	6.50	118.40	109.18
1	B	365	THR	N-CA-C	6.32	118.16	109.18
1	A	243	ASN	CB-CA-C	-6.25	106.76	111.20
1	B	441	TRP	N-CA-C	6.23	119.31	109.96
1	D	364	HIS	N-CA-C	-6.14	99.99	109.76
1	F	542	ASP	N-CA-C	-6.12	100.74	109.24
1	A	455	LEU	N-CA-C	6.00	119.15	110.28
1	B	498	ARG	N-CA-C	5.98	118.28	111.11
1	E	441	TRP	N-CA-C	5.93	118.85	109.96
1	C	364	HIS	N-CA-C	-5.82	100.50	109.76
1	A	542	ASP	N-CA-C	-5.82	101.15	109.24
1	A	364	HIS	N-CA-C	-5.81	100.52	109.76
1	C	498	ARG	N-CA-C	5.81	118.08	111.11
1	D	441	TRP	N-CA-C	5.80	118.67	109.96
1	A	441	TRP	N-CA-C	5.79	118.65	109.96
1	E	364	HIS	N-CA-C	-5.79	100.55	109.76
1	C	441	TRP	N-CA-C	5.76	118.69	110.10
1	A	498	ARG	N-CA-C	5.65	118.17	111.33
1	D	455	LEU	N-CA-C	5.65	118.65	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	HIS	N-CA-C	-5.59	100.88	109.76
1	F	498	ARG	N-CA-C	5.58	117.81	111.11
1	C	455	LEU	N-CA-C	5.58	118.53	110.28
1	D	498	ARG	N-CA-C	5.55	117.77	111.11
1	E	455	LEU	N-CA-C	5.53	118.47	110.28
1	B	363	SER	N-CA-C	5.50	117.05	110.44
1	F	410	ASP	N-CA-C	5.45	119.49	112.41
1	A	363	SER	N-CA-C	5.43	116.95	110.44
1	E	498	ARG	N-CA-C	5.39	117.58	111.11
1	E	399	GLN	N-CA-C	5.36	117.21	111.36
1	F	441	TRP	N-CA-C	5.36	117.99	109.96
1	D	399	GLN	N-CA-C	5.28	117.11	111.36
1	B	399	GLN	N-CA-C	5.28	117.11	111.36
1	C	399	GLN	N-CA-C	5.26	117.09	111.36
1	A	537	HIS	N-CA-C	5.23	118.92	112.54
1	B	532	ALA	N-CA-C	5.19	117.59	108.56
1	C	168	ASP	CA-C-N	5.18	124.98	119.28
1	C	168	ASP	C-N-CA	5.18	124.98	119.28
1	C	410	ASP	N-CA-C	5.17	119.13	112.41
1	C	537	HIS	N-CA-C	5.17	118.84	112.54
1	D	243	ASN	CB-CA-C	-5.17	107.53	111.20
1	F	317	ILE	N-CA-C	5.16	115.34	108.11
1	E	537	HIS	N-CA-C	5.13	118.80	112.54
1	F	456	THR	N-CA-C	-5.13	106.43	113.30
1	D	317	ILE	N-CA-C	5.11	115.33	108.17
1	A	532	ALA	N-CA-C	5.10	117.43	108.56
1	F	217	TYR	N-CA-C	5.06	118.94	112.87
1	B	455	LEU	N-CA-C	5.04	117.75	110.28
1	F	399	GLN	N-CA-C	5.04	116.85	111.36
1	B	317	ILE	N-CA-C	5.03	115.16	108.11
1	A	399	GLN	N-CA-C	5.02	116.83	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	TYR	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	A	3559	0	3376	39	0
1	B	3552	0	3367	41	0
1	C	3559	0	3376	37	0
1	D	3552	0	3367	36	0
1	E	3552	0	3367	38	0
1	F	3552	0	3367	45	0
2	H	54	0	53	0	0
2	I	54	0	53	0	0
2	J	54	0	53	0	0
2	K	54	0	53	0	0
2	L	54	0	53	0	0
2	N	54	0	53	0	0
3	A	12	0	4	0	0
3	B	12	0	4	0	0
3	C	12	0	4	0	0
3	D	12	0	4	0	0
3	E	12	0	4	0	0
3	F	12	0	4	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	244	0	0	3	0
6	B	216	0	0	0	0
6	C	236	0	0	4	0
6	D	218	0	0	3	0
6	E	209	0	0	3	0
6	F	193	0	0	2	0
6	H	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	5	0	0	0	0
6	J	6	0	0	0	0
6	K	5	0	0	0	0
6	L	3	0	0	0	0
6	N	6	0	0	0	0
All	All	23092	0	20562	234	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 6.

All (234) 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:E:479:ASN:HD22	1:E:479:ASN:H	0.98	0.95
1:A:479:ASN:H	1:A:479:ASN:HD22	1.13	0.92
1:D:479:ASN:H	1:D:479:ASN:HD22	1.05	0.92
1:D:479:ASN:H	1:D:479:ASN:ND2	1.67	0.92
1:B:479:ASN:HD22	1:B:479:ASN:H	1.18	0.91
1:E:178:GLN:HE22	1:E:238:ARG:HH22	1.09	0.90
1:D:479:ASN:HB3	6:D:845:HOH:O	1.74	0.85
1:E:479:ASN:H	1:E:479:ASN:ND2	1.74	0.85
1:F:479:ASN:H	1:F:479:ASN:HD22	1.24	0.85
1:A:479:ASN:HB3	6:A:871:HOH:O	1.77	0.84
1:A:479:ASN:H	1:A:479:ASN:ND2	1.71	0.83
1:E:178:GLN:HE22	1:E:238:ARG:NH2	1.78	0.81
1:C:454:ILE:HD12	1:C:469:LYS:HG2	1.61	0.81
1:C:126:GLY:HA3	6:C:853:HOH:O	1.84	0.78
1:B:479:ASN:H	1:B:479:ASN:ND2	1.78	0.78
1:E:477:GLU:HG2	6:E:856:HOH:O	1.83	0.77
1:F:479:ASN:H	1:F:479:ASN:ND2	1.83	0.77
1:E:479:ASN:HD22	1:E:479:ASN:N	1.74	0.73
1:D:479:ASN:HD22	1:D:479:ASN:N	1.78	0.73
1:E:178:GLN:NE2	1:E:238:ARG:HH22	1.86	0.71
1:A:479:ASN:HD22	1:A:479:ASN:N	1.83	0.71
1:B:463:LYS:HE2	1:B:553:ASN:O	1.91	0.70
1:B:479:ASN:HD22	1:B:479:ASN:N	1.84	0.70
1:A:259:ASP:OD1	1:A:262:THR:HG23	1.93	0.68
1:D:454:ILE:HD12	1:D:469:LYS:HG2	1.76	0.67
1:D:193:ARG:HA	1:D:356:LEU:HG	1.77	0.66
1:A:418:ARG:NH1	1:A:540:ASP:OD2	2.28	0.66
1:A:479:ASN:ND2	1:A:479:ASN:N	2.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:ASN:HB3	6:E:848:HOH:O	1.97	0.65
1:E:454:ILE:HD12	1:E:469:LYS:HG2	1.79	0.65
1:A:523:TYR:HD1	1:A:523:TYR:H	1.42	0.63
1:D:233:ASP:CG	1:D:267:ALA:HB3	2.25	0.62
1:D:479:ASN:ND2	1:D:479:ASN:N	2.37	0.62
1:A:206:ALA:HA	1:A:213:VAL:HG12	1.82	0.61
1:F:233:ASP:CG	1:F:267:ALA:HB3	2.25	0.61
1:A:512:ARG:NH2	1:A:550:GLU:OE2	2.33	0.61
1:B:233:ASP:CG	1:B:267:ALA:HB3	2.26	0.60
1:B:463:LYS:O	1:B:463:LYS:HD3	2.00	0.60
1:F:352:VAL:HG22	1:F:362:GLU:HG2	1.82	0.60
1:A:404:ALA:O	1:A:405:HIS:HB2	2.00	0.60
1:B:479:ASN:ND2	1:B:479:ASN:N	2.46	0.60
1:B:493:LEU:HD12	1:B:493:LEU:C	2.27	0.59
1:A:259:ASP:OD1	1:A:262:THR:CG2	2.50	0.59
1:F:404:ALA:O	1:F:405:HIS:HB2	2.03	0.58
1:E:468:ARG:HG2	1:E:548:VAL:HG22	1.86	0.58
1:A:523:TYR:CD1	1:A:523:TYR:N	2.67	0.58
1:C:333:CYS:HA	6:C:749:HOH:O	2.04	0.58
1:C:454:ILE:CD1	1:C:469:LYS:HG2	2.34	0.57
1:E:404:ALA:O	1:E:405:HIS:HB2	2.04	0.57
1:C:233:ASP:CG	1:C:267:ALA:HB3	2.29	0.57
1:F:186:TYR:CE2	1:F:356:LEU:HD22	2.39	0.57
1:F:298:ARG:HD2	1:F:299:GLU:OE2	2.03	0.57
1:C:295:ASN:OD1	1:C:367:THR:HG22	2.05	0.56
1:F:468:ARG:HG2	1:F:548:VAL:HG22	1.88	0.56
1:B:418:ARG:NH1	1:B:540:ASP:OD2	2.38	0.56
1:F:484:LEU:HD23	1:F:571:TYR:O	2.05	0.56
1:A:118:PHE:HB3	1:A:119:PRO:HD3	1.87	0.56
1:C:128:THR:O	1:C:130:ARG:HG2	2.06	0.56
1:D:341:TYR:CE2	1:D:428:LEU:HD21	2.41	0.56
1:F:479:ASN:HB3	6:F:828:HOH:O	2.06	0.55
1:C:351:ILE:HG13	1:C:369:ALA:HB1	1.88	0.55
1:C:295:ASN:CG	1:C:367:THR:HG22	2.32	0.55
1:E:193:ARG:HE	1:E:197:ARG:CZ	2.20	0.55
1:E:233:ASP:CG	1:E:267:ALA:HB3	2.32	0.55
1:A:464:ARG:NH2	1:A:466:GLU:OE2	2.40	0.55
1:A:128:THR:O	1:A:130:ARG:HG2	2.06	0.54
1:B:295:ASN:CG	1:B:367:THR:HG22	2.33	0.54
1:D:186:TYR:CE2	1:D:356:LEU:HD22	2.42	0.54
1:D:206:ALA:HA	1:D:213:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:HIS:CD2	1:B:358:GLN:HA	2.42	0.54
1:A:523:TYR:HD1	1:A:523:TYR:N	2.03	0.53
1:F:186:TYR:HE2	1:F:356:LEU:HD22	1.72	0.53
1:F:479:ASN:HD22	1:F:479:ASN:N	1.91	0.53
1:B:454:ILE:HD11	1:B:568:LEU:HB2	1.91	0.53
1:D:295:ASN:OD1	1:D:367:THR:HG22	2.08	0.53
1:E:493:LEU:C	1:E:493:LEU:HD12	2.33	0.53
1:F:293:SER:HA	1:F:309:THR:HG21	1.91	0.53
1:F:295:ASN:OD1	1:F:367:THR:HG22	2.09	0.53
1:B:508:PRO:HD3	1:B:547:TRP:CE2	2.44	0.52
1:B:234:ALA:O	1:B:238:ARG:HG3	2.09	0.52
1:E:295:ASN:CG	1:E:367:THR:HG22	2.33	0.52
1:F:418:ARG:NH1	1:F:540:ASP:OD2	2.42	0.52
1:C:468:ARG:HG2	1:C:548:VAL:HG22	1.92	0.52
1:B:463:LYS:HD3	1:B:463:LYS:C	2.36	0.51
1:D:295:ASN:CG	1:D:367:THR:HG22	2.35	0.51
1:F:464:ARG:NH2	1:F:466:GLU:OE2	2.43	0.51
1:A:233:ASP:CG	1:A:267:ALA:HB3	2.35	0.51
1:E:160:HIS:CD2	1:E:358:GLN:HA	2.45	0.51
1:A:193:ARG:NH1	6:A:880:HOH:O	2.44	0.51
1:A:160:HIS:CD2	1:A:358:GLN:HA	2.46	0.51
1:B:341:TYR:CZ	1:B:428:LEU:HD21	2.46	0.51
1:F:282:ARG:HD3	1:F:286:GLY:O	2.10	0.51
1:C:463:LYS:O	1:C:463:LYS:HD3	2.12	0.50
1:F:295:ASN:CG	1:F:367:THR:HG22	2.37	0.50
1:A:493:LEU:C	1:A:493:LEU:HD12	2.36	0.50
6:A:864:HOH:O	1:B:268:ARG:HD3	2.11	0.50
1:D:457:GLU:OE2	1:D:459:LYS:HE3	2.10	0.50
1:D:458:PRO:HG3	6:D:883:HOH:O	2.11	0.50
1:C:404:ALA:O	1:C:405:HIS:HB2	2.12	0.50
1:D:418:ARG:NH1	1:D:540:ASP:OD2	2.45	0.50
1:E:298:ARG:HG2	1:E:299:GLU:OE2	2.12	0.50
1:F:479:ASN:ND2	1:F:479:ASN:N	2.49	0.50
1:B:404:ALA:O	1:B:405:HIS:HB2	2.12	0.49
1:D:404:ALA:O	1:D:405:HIS:HB2	2.10	0.49
1:D:282:ARG:HD3	1:D:286:GLY:O	2.11	0.49
1:C:493:LEU:C	1:C:493:LEU:HD12	2.37	0.49
1:A:371:ALA:HB3	1:A:372:PRO:HD3	1.95	0.49
1:E:298:ARG:HB3	6:E:844:HOH:O	2.13	0.49
1:C:512:ARG:NH1	1:C:550:GLU:OE2	2.38	0.49
1:D:371:ALA:HB3	1:D:372:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:539:TRP:O	1:E:540:ASP:HB2	2.14	0.48
1:E:272:GLU:O	1:E:276:ARG:HG3	2.12	0.48
1:E:479:ASN:ND2	1:E:479:ASN:N	2.44	0.48
1:C:468:ARG:NH2	1:C:546:GLU:OE2	2.46	0.48
1:E:351:ILE:HG13	1:E:369:ALA:HB1	1.95	0.48
1:A:298:ARG:HD2	1:A:299:GLU:OE2	2.14	0.47
1:D:351:ILE:HG13	1:D:369:ALA:HB1	1.96	0.47
1:F:341:TYR:CZ	1:F:428:LEU:HD21	2.50	0.47
1:F:351:ILE:HG13	1:F:369:ALA:HB1	1.96	0.47
1:F:508:PRO:HD3	1:F:547:TRP:CE2	2.50	0.47
1:F:539:TRP:O	1:F:540:ASP:HB2	2.13	0.47
1:A:539:TRP:O	1:A:540:ASP:HB2	2.14	0.47
1:E:418:ARG:NH1	1:E:540:ASP:OD2	2.40	0.46
1:B:351:ILE:HB	1:B:364:HIS:HB3	1.96	0.46
1:C:351:ILE:HB	1:C:364:HIS:HB3	1.96	0.46
1:F:118:PHE:N	1:F:119:PRO:CD	2.78	0.46
1:A:282:ARG:HD3	1:A:286:GLY:O	2.16	0.46
1:B:341:TYR:CE2	1:B:428:LEU:HD21	2.51	0.46
1:D:458:PRO:O	1:D:459:LYS:HD2	2.15	0.46
1:E:448:ARG:HD3	1:E:479:ASN:HA	1.98	0.46
1:A:508:PRO:HD3	1:A:547:TRP:CE2	2.50	0.46
1:F:463:LYS:NZ	1:F:555:SER:O	2.49	0.46
1:C:117:LYS:HD2	1:C:120:GLN:OE1	2.16	0.46
1:C:293:SER:HA	1:C:309:THR:HG21	1.98	0.46
1:D:118:PHE:HB3	1:D:119:PRO:HD3	1.99	0.46
1:A:293:SER:HA	1:A:309:THR:HG21	1.98	0.45
1:B:295:ASN:OD1	1:B:367:THR:HG22	2.15	0.45
1:C:272:GLU:O	1:C:276:ARG:HG3	2.16	0.45
1:C:480:HIS:HE1	6:C:864:HOH:O	2.00	0.45
1:D:341:TYR:CZ	1:D:428:LEU:HD21	2.51	0.45
1:F:493:LEU:C	1:F:493:LEU:HD12	2.42	0.45
1:B:539:TRP:O	1:B:540:ASP:HB2	2.15	0.45
1:C:160:HIS:CD2	1:C:358:GLN:HA	2.52	0.45
1:F:333:CYS:HA	6:F:749:HOH:O	2.15	0.45
1:C:539:TRP:O	1:C:540:ASP:HB2	2.16	0.45
1:B:117:LYS:HD2	1:B:120:GLN:OE1	2.16	0.45
1:C:172:SER:HB3	1:C:182:PRO:HG3	1.98	0.45
1:F:351:ILE:HB	1:F:364:HIS:HB3	1.98	0.45
1:A:404:ALA:O	1:A:405:HIS:CB	2.65	0.44
1:F:402:LYS:HA	1:F:403:PRO:HD3	1.86	0.44
1:A:295:ASN:CG	1:A:367:THR:HG22	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASN:N	1:B:244:PRO:HD3	2.32	0.44
1:A:566:PHE:CD1	1:A:566:PHE:C	2.93	0.44
1:C:118:PHE:N	1:C:119:PRO:CD	2.80	0.44
1:E:329:TYR:CZ	1:E:366:GLY:HA2	2.53	0.44
1:B:477:GLU:HB3	1:B:478:PRO:CD	2.48	0.44
1:E:233:ASP:OD2	1:E:269:LEU:HB2	2.18	0.44
1:C:463:LYS:HD3	1:C:463:LYS:C	2.43	0.44
1:F:371:ALA:HB3	1:F:372:PRO:HD3	1.99	0.44
1:D:351:ILE:HB	1:D:364:HIS:HB3	1.99	0.44
1:C:508:PRO:HD3	1:C:547:TRP:CE2	2.53	0.43
1:F:497:ARG:HD2	1:F:500:ASP:OD2	2.17	0.43
1:D:493:LEU:HD12	1:D:493:LEU:C	2.43	0.43
1:F:304:ASN:OD1	1:F:333:CYS:HB2	2.18	0.43
1:F:382:LEU:HD23	1:F:382:LEU:HA	1.82	0.43
1:A:458:PRO:O	1:A:459:LYS:HD2	2.18	0.43
1:E:282:ARG:HD3	1:E:286:GLY:O	2.18	0.43
1:E:508:PRO:HD3	1:E:547:TRP:CE2	2.53	0.43
1:E:341:TYR:CZ	1:E:428:LEU:HD21	2.54	0.43
1:D:512:ARG:NH1	1:D:550:GLU:OE1	2.49	0.43
1:E:118:PHE:N	1:E:119:PRO:CD	2.81	0.43
1:A:304:ASN:CG	1:A:333:CYS:HB2	2.44	0.43
1:B:168:ASP:OD1	1:B:168:ASP:C	2.62	0.43
1:A:468:ARG:HG2	1:A:548:VAL:HG22	1.99	0.43
1:E:395:HIS:CD2	1:E:444:VAL:HG11	2.54	0.43
1:A:454:ILE:HD12	1:A:469:LYS:HG2	2.00	0.43
1:D:539:TRP:O	1:D:540:ASP:HB2	2.18	0.43
1:E:295:ASN:ND2	1:E:367:THR:HG22	2.34	0.42
1:A:351:ILE:HB	1:A:364:HIS:HB3	2.01	0.42
1:D:329:TYR:CZ	1:D:366:GLY:HA2	2.54	0.42
1:F:341:TYR:CE2	1:F:428:LEU:HD21	2.54	0.42
1:C:153:ASP:CG	1:C:194:HIS:HD1	2.27	0.42
1:C:404:ALA:O	1:C:405:HIS:CB	2.67	0.42
1:B:153:ASP:CG	1:B:194:HIS:HD1	2.27	0.42
1:B:382:LEU:HD23	1:B:382:LEU:HA	1.92	0.42
1:B:404:ALA:O	1:B:405:HIS:CB	2.67	0.42
1:B:458:PRO:O	1:B:459:LYS:HD2	2.19	0.42
1:C:345:ASN:HB2	1:F:326:VAL:O	2.19	0.42
1:C:458:PRO:HG3	6:C:889:HOH:O	2.19	0.42
1:D:160:HIS:CD2	1:D:358:GLN:HA	2.54	0.42
1:A:351:ILE:HG13	1:A:369:ALA:HB1	2.02	0.42
1:E:295:ASN:OD1	1:E:367:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TYR:CE1	1:B:384:ALA:HA	2.55	0.42
1:F:160:HIS:CD2	1:F:358:GLN:HA	2.55	0.42
1:B:118:PHE:HB3	1:B:119:PRO:HD3	2.02	0.42
1:B:232:THR:OG1	1:B:235:VAL:HG23	2.20	0.42
1:C:154:ASP:OD2	1:C:192:ASN:HA	2.20	0.42
1:D:468:ARG:HG2	1:D:548:VAL:HG22	2.02	0.42
1:B:206:ALA:HA	1:B:213:VAL:HG12	2.02	0.41
1:E:512:ARG:HH22	1:E:550:GLU:CD	2.25	0.41
1:F:172:SER:HB3	1:F:182:PRO:HG3	2.02	0.41
1:C:326:VAL:O	1:F:345:ASN:HB2	2.20	0.41
1:F:113:PRO:HB3	1:F:213:VAL:HG11	2.02	0.41
1:A:259:ASP:CG	1:A:262:THR:CG2	2.94	0.41
1:C:142:TYR:CE1	1:C:384:ALA:HA	2.56	0.41
1:A:172:SER:HB3	1:A:182:PRO:HG3	2.03	0.41
1:B:183:GLN:HA	1:B:184:PRO:HD3	1.94	0.41
1:D:288:ILE:HG21	1:D:378:ILE:HG21	2.03	0.41
1:D:333:CYS:HA	6:D:731:HOH:O	2.21	0.41
1:E:371:ALA:HB3	1:E:372:PRO:HD3	2.02	0.41
1:E:495:TYR:OH	1:E:559:ASN:HB2	2.20	0.41
1:F:168:ASP:OD1	1:F:168:ASP:C	2.64	0.41
1:F:454:ILE:HD12	1:F:566:PHE:CE2	2.56	0.41
1:B:293:SER:HA	1:B:309:THR:HG21	2.03	0.41
1:B:403:PRO:HB3	1:B:411:TRP:CH2	2.56	0.41
1:C:341:TYR:CE2	1:C:428:LEU:HD21	2.56	0.41
1:D:404:ALA:O	1:D:405:HIS:CB	2.67	0.41
1:F:475:LEU:HA	1:F:480:HIS:ND1	2.35	0.41
1:B:482:THR:OG1	1:B:574:ALA:HA	2.20	0.41
1:B:512:ARG:NH1	1:B:550:GLU:OE1	2.50	0.41
1:D:497:ARG:HD2	1:D:500:ASP:OD2	2.21	0.41
1:E:341:TYR:CE2	1:E:428:LEU:HD21	2.55	0.40
1:E:351:ILE:HB	1:E:364:HIS:HB3	2.03	0.40
1:F:143:THR:OG1	1:F:218:ASN:HB2	2.20	0.40
1:C:113:PRO:HB3	1:C:213:VAL:HG11	2.02	0.40
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.93	0.40
1:F:495:TYR:OH	1:F:559:ASN:HB2	2.21	0.40
1:A:329:TYR:CZ	1:A:366:GLY:HA2	2.56	0.40
1:C:484:LEU:HD23	1:C:571:TYR:O	2.22	0.40
1:F:243:ASN:N	1:F:244:PRO:HD3	2.37	0.40
1:B:118:PHE:N	1:B:119:PRO:CD	2.85	0.40
1:C:496:ASN:OD1	1:C:559:ASN:HB3	2.21	0.40
1:D:272:GLU:O	1:D:276:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ILE:HD13	1:B:566:PHE:CE2	2.56	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	A	464/482 (96%)	446 (96%)	18 (4%)	0	100	100
1	B	463/482 (96%)	444 (96%)	19 (4%)	0	100	100
1	C	464/482 (96%)	443 (96%)	21 (4%)	0	100	100
1	D	463/482 (96%)	443 (96%)	20 (4%)	0	100	100
1	E	463/482 (96%)	442 (96%)	21 (4%)	0	100	100
1	F	463/482 (96%)	444 (96%)	19 (4%)	0	100	100
2	H	1/5 (20%)	1 (100%)	0	0	100	100
2	I	1/5 (20%)	1 (100%)	0	0	100	100
2	J	1/5 (20%)	1 (100%)	0	0	100	100
2	K	1/5 (20%)	1 (100%)	0	0	100	100
2	L	1/5 (20%)	1 (100%)	0	0	100	100
2	N	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2786/2922 (95%)	2668 (96%)	118 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/390 (96%)	365 (97%)	11 (3%)	37	55
1	B	375/390 (96%)	370 (99%)	5 (1%)	61	77
1	C	376/390 (96%)	369 (98%)	7 (2%)	50	69
1	D	375/390 (96%)	367 (98%)	8 (2%)	47	66
1	E	375/390 (96%)	363 (97%)	12 (3%)	34	51
1	F	375/390 (96%)	367 (98%)	8 (2%)	47	66
2	H	3/3 (100%)	3 (100%)	0	100	100
2	I	3/3 (100%)	3 (100%)	0	100	100
2	J	3/3 (100%)	3 (100%)	0	100	100
2	K	3/3 (100%)	3 (100%)	0	100	100
2	L	3/3 (100%)	3 (100%)	0	100	100
2	N	3/3 (100%)	3 (100%)	0	100	100
All	All	2270/2358 (96%)	2219 (98%)	51 (2%)	45	65

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	178	GLN
1	A	262	THR
1	A	298	ARG
1	A	420	VAL
1	A	428	LEU
1	A	479	ASN
1	A	497	ARG
1	A	523	TYR
1	A	555	SER
1	A	565	LYS
1	B	243	ASN
1	B	435	VAL
1	B	463	LYS
1	B	479	ASN
1	B	565	LYS
1	C	178	GLN
1	C	230	GLU

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Mol	Chain	Res	Type
1	C	406	LEU
1	C	463	LYS
1	C	484	LEU
1	C	555	SER
1	C	565	LYS
1	D	178	GLN
1	D	182	PRO
1	D	387	ASN
1	D	406	LEU
1	D	420	VAL
1	D	457	GLU
1	D	479	ASN
1	D	565	LYS
1	E	134	VAL
1	E	188	GLN
1	E	230	GLU
1	E	298	ARG
1	E	303	CYS
1	E	406	LEU
1	E	435	VAL
1	E	479	ASN
1	E	483	ARG
1	E	497	ARG
1	E	555	SER
1	E	565	LYS
1	F	356	LEU
1	F	406	LEU
1	F	419	LYS
1	F	420	VAL
1	F	459	LYS
1	F	479	ASN
1	F	484	LEU
1	F	565	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	300	HIS
1	A	346	GLN
1	A	387	ASN
1	A	479	ASN

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Mol	Chain	Res	Type
1	A	488	GLN
1	B	243	ASN
1	B	325	ASN
1	B	346	GLN
1	B	387	ASN
1	B	479	ASN
1	C	140	GLN
1	C	243	ASN
1	C	300	HIS
1	C	325	ASN
1	C	346	GLN
1	C	387	ASN
1	C	480	HIS
1	C	488	GLN
1	D	300	HIS
1	D	346	GLN
1	D	479	ASN
1	D	488	GLN
1	E	178	GLN
1	E	188	GLN
1	E	243	ASN
1	E	300	HIS
1	E	364	HIS
1	E	387	ASN
1	E	479	ASN
1	F	243	ASN
1	F	300	HIS
1	F	325	ASN
1	F	346	GLN
1	F	387	ASN
1	F	479	ASN
1	F	504	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	$\# Z > 2$
3	FMT	C	601	-	2,2,2	0.62	0	1,1,1	0.02	0
3	FMT	E	601	-	2,2,2	0.53	0	1,1,1	0.05	0
3	FMT	A	602	-	2,2,2	0.50	0	1,1,1	0.06	0
3	FMT	D	603	-	2,2,2	0.54	0	1,1,1	0.07	0
3	FMT	A	604	-	2,2,2	0.56	0	1,1,1	0.06	0
3	FMT	A	603	-	2,2,2	0.71	0	1,1,1	0.02	0
3	FMT	B	601	-	2,2,2	0.75	0	1,1,1	0.01	0
3	FMT	F	602	-	2,2,2	0.56	0	1,1,1	0.05	0
3	FMT	F	603	-	2,2,2	0.48	0	1,1,1	0.06	0
3	FMT	E	604	-	2,2,2	0.58	0	1,1,1	0.05	0
3	FMT	D	604	-	2,2,2	0.54	0	1,1,1	0.08	0
3	FMT	D	602	-	2,2,2	0.58	0	1,1,1	0.06	0
3	FMT	B	602	-	2,2,2	0.55	0	1,1,1	0.06	0
3	FMT	F	604	-	2,2,2	0.48	0	1,1,1	0.08	0
3	FMT	B	603	-	2,2,2	0.55	0	1,1,1	0.05	0
3	FMT	E	602	-	2,2,2	0.47	0	1,1,1	0.08	0
3	FMT	C	604	-	2,2,2	0.54	0	1,1,1	0.07	0
3	FMT	D	601	-	2,2,2	0.58	0	1,1,1	0.04	0
3	FMT	A	601	-	2,2,2	0.55	0	1,1,1	0.05	0
3	FMT	C	602	-	2,2,2	0.51	0	1,1,1	0.06	0
3	FMT	E	603	-	2,2,2	0.66	0	1,1,1	0.04	0
3	FMT	B	604	-	2,2,2	0.50	0	1,1,1	0.07	0
3	FMT	C	603	-	2,2,2	0.69	0	1,1,1	0.02	0
3	FMT	F	601	-	2,2,2	0.70	0	1,1,1	0.02	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	466/482 (96%)	-0.49	10 (2%) 63 65	14, 22, 38, 64	13 (2%)
1	B	465/482 (96%)	-0.46	11 (2%) 59 62	13, 24, 40, 69	15 (3%)
1	C	466/482 (96%)	-0.52	10 (2%) 63 65	14, 22, 38, 54	14 (3%)
1	D	465/482 (96%)	-0.42	9 (1%) 66 68	13, 24, 40, 65	18 (3%)
1	E	465/482 (96%)	-0.40	12 (2%) 57 59	9, 24, 41, 75	13 (2%)
1	F	465/482 (96%)	-0.31	12 (2%) 57 59	13, 27, 44, 70	19 (4%)
2	H	3/5 (60%)	-0.77	0 100 100	20, 20, 20, 22	0
2	I	3/5 (60%)	-0.66	0 100 100	24, 24, 26, 27	0
2	J	3/5 (60%)	-0.87	0 100 100	25, 25, 26, 26	0
2	K	3/5 (60%)	-1.02	0 100 100	18, 18, 19, 21	0
2	L	3/5 (60%)	-0.54	0 100 100	22, 22, 24, 27	0
2	N	3/5 (60%)	-0.95	0 100 100	21, 21, 22, 23	0
All	All	2810/2922 (96%)	-0.43	64 (2%) 61 63	9, 24, 41, 75	92 (3%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	VAL	8.3
1	D	127	VAL	8.2
1	E	127	VAL	7.2
1	F	127	VAL	7.2
1	B	127	VAL	6.8
1	C	128	THR	6.4
1	C	127	VAL	6.4
1	D	129	GLN	6.4
1	F	128	THR	6.3
1	A	128	THR	6.2
1	A	129	GLN	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	128	THR	5.9
1	C	129	GLN	5.8
1	E	128	THR	5.6
1	B	128	THR	5.6
1	E	129	GLN	5.5
1	E	110	TYR	5.2
1	F	129	GLN	4.6
1	B	129	GLN	4.5
1	F	110	TYR	3.7
1	E	111	GLN	3.5
1	F	440	ASN	3.5
1	F	404	ALA	3.4
1	B	126	GLY	3.3
1	B	440	ASN	3.3
1	E	440	ASN	3.2
1	A	440	ASN	3.1
1	C	440	ASN	3.0
1	D	574	ALA	2.9
1	C	405	HIS	2.8
1	E	126	GLY	2.7
1	E	130	ARG	2.6
1	D	405	HIS	2.6
1	E	405	HIS	2.6
1	F	574	ALA	2.6
1	A	130	ARG	2.6
1	D	126	GLY	2.6
1	A	126	GLY	2.5
1	F	126	GLY	2.5
1	F	405	HIS	2.5
1	C	126	GLY	2.5
1	B	130	ARG	2.4
1	D	404	ALA	2.4
1	E	404	ALA	2.4
1	B	558	ASN	2.3
1	C	130	ARG	2.3
1	F	111	GLN	2.3
1	C	404	ALA	2.3
1	D	440	ASN	2.3
1	B	189	MET	2.3
1	F	523	TYR	2.3
1	B	111	GLN	2.2
1	B	405	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	125	SER	2.2
1	C	109	VAL	2.2
1	E	189	MET	2.2
1	A	523	TYR	2.2
1	A	109	VAL	2.1
1	A	405	HIS	2.1
1	C	189	MET	2.1
1	A	574	ALA	2.1
1	D	523	TYR	2.1
1	B	462	GLY	2.0
1	F	130	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FMT	B	601	3/3	0.81	0.15	27,27,28,34	0
3	FMT	E	601	3/3	0.83	0.14	39,39,40,42	0
3	FMT	B	604	3/3	0.84	0.12	39,39,40,43	0
3	FMT	A	603	3/3	0.86	0.12	27,27,32,36	0
3	FMT	B	603	3/3	0.86	0.12	40,40,41,41	0
3	FMT	C	603	3/3	0.88	0.11	23,23,23,28	0
3	FMT	D	603	3/3	0.90	0.09	37,37,37,37	0
3	FMT	F	601	3/3	0.90	0.10	25,25,37,37	0
3	FMT	D	601	3/3	0.91	0.10	28,28,32,34	0
3	FMT	C	602	3/3	0.91	0.10	34,34,35,35	0
3	FMT	A	601	3/3	0.92	0.10	35,35,38,39	0
3	FMT	E	603	3/3	0.92	0.10	22,22,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMT	C	601	3/3	0.92	0.10	29,29,33,36	0
3	FMT	F	603	3/3	0.92	0.11	36,36,38,39	0
3	FMT	E	602	3/3	0.93	0.09	34,34,36,40	0
3	FMT	F	604	3/3	0.94	0.09	35,35,38,42	0
3	FMT	A	602	3/3	0.95	0.06	36,36,37,37	0
3	FMT	D	604	3/3	0.95	0.08	34,34,35,37	0
3	FMT	D	602	3/3	0.96	0.06	23,23,25,27	0
3	FMT	C	604	3/3	0.98	0.05	25,25,25,26	0
3	FMT	F	602	3/3	0.98	0.05	23,23,27,28	0
4	CA	E	605	1/1	0.98	0.03	29,29,29,29	0
4	CA	E	607	1/1	0.98	0.03	35,35,35,35	0
5	NA	E	608	1/1	0.98	0.06	19,19,19,19	0
4	CA	B	605	1/1	0.99	0.02	26,26,26,26	0
4	CA	B	606	1/1	0.99	0.02	17,17,17,17	0
4	CA	B	607	1/1	0.99	0.03	38,38,38,38	0
4	CA	C	605	1/1	0.99	0.01	18,18,18,18	0
4	CA	C	606	1/1	0.99	0.01	20,20,20,20	0
4	CA	C	607	1/1	0.99	0.04	31,31,31,31	0
4	CA	D	605	1/1	0.99	0.03	24,24,24,24	0
3	FMT	A	604	3/3	0.99	0.03	24,24,27,29	0
3	FMT	E	604	3/3	0.99	0.02	18,18,21,21	0
4	CA	F	605	1/1	0.99	0.02	27,27,27,27	0
4	CA	F	607	1/1	0.99	0.03	33,33,33,33	0
5	NA	A	608	1/1	0.99	0.02	17,17,17,17	0
5	NA	B	608	1/1	0.99	0.02	18,18,18,18	0
5	NA	C	608	1/1	0.99	0.02	17,17,17,17	0
5	NA	D	608	1/1	0.99	0.04	17,17,17,17	0
3	FMT	B	602	3/3	0.99	0.05	20,20,21,22	0
5	NA	F	608	1/1	0.99	0.04	16,16,16,16	0
4	CA	D	606	1/1	1.00	0.01	16,16,16,16	0
4	CA	D	607	1/1	1.00	0.02	25,25,25,25	0
4	CA	A	606	1/1	1.00	0.01	16,16,16,16	0
4	CA	E	606	1/1	1.00	0.02	16,16,16,16	0
4	CA	A	607	1/1	1.00	0.02	32,32,32,32	0
4	CA	A	605	1/1	1.00	0.01	21,21,21,21	0
4	CA	F	606	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers

There are no such residues in this entry.