



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:56 PM UTC

PDB ID : 4OMD / pdb_00004omd
Title : X-ray structure of human furin in complex with the competitive inhibitor Phac-RVR-Amba
Authors : Dahms, S.O.; Than, M.E.
Deposited on : 2014-01-27
Resolution : 2.70 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

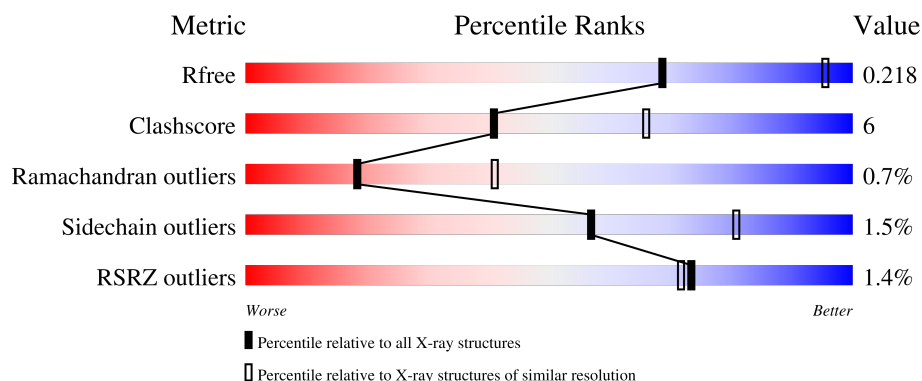
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	
1	B	482	
1	C	482	
1	D	482	
1	E	482	

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Mol	Chain	Length	Quality of chain
1	F	482	% 78% 17% • •
2	H	5	100%
2	I	5	80% 20%
2	J	5	100%
2	K	5	80% 20%
2	L	5	80% 20%
2	N	5	80% 20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22341 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 phenylacetyl-Arg-Val-Arg-(amidomethyl)benzamidine.

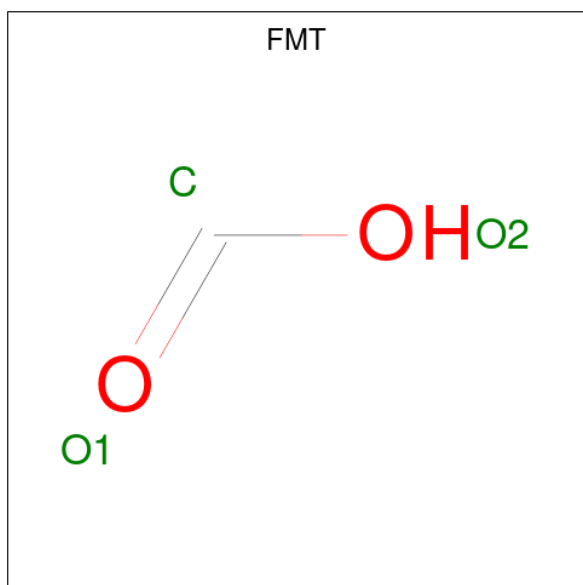
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	5	Total	C	N	O	6	0	0
			49	33	12	4			
2	I	5	Total	C	N	O	6	0	0
			49	33	12	4			
2	J	5	Total	C	N	O	6	0	0
			49	33	12	4			
2	K	5	Total	C	N	O	6	0	0
			49	33	12	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	5	Total	C	N	O	6	0	0
			49	33	12	4			
2	N	5	Total	C	N	O	6	0	0
			49	33	12	4			

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

- 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
4	D	3	Total Ca 3 3	0	0
4	E	3	Total Ca 3 3	0	0
4	F	3	Total Ca 3 3	0	0

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

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

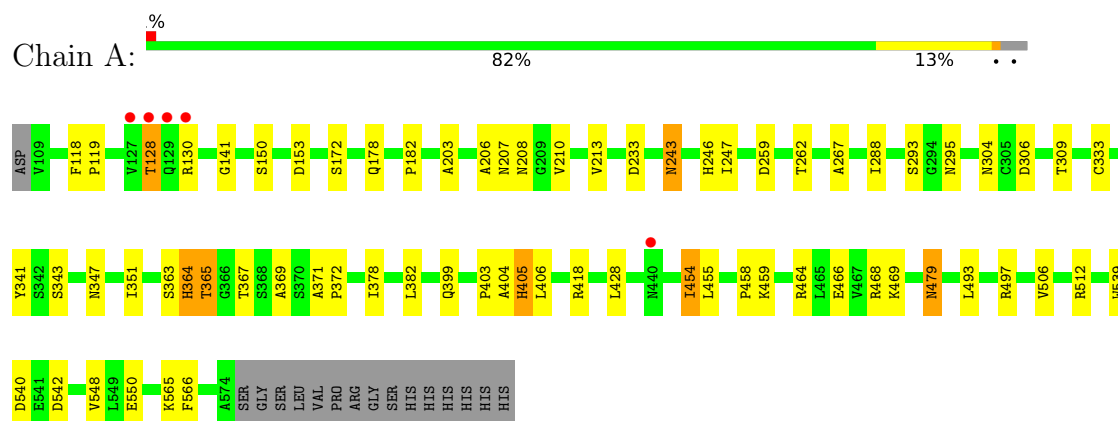
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total 112	O 112	0	0
6	B	96	Total 96	O 96	0	0
6	C	113	Total 113	O 113	0	0
6	D	125	Total 125	O 125	0	0
6	E	106	Total 106	O 106	0	0
6	F	94	Total 94	O 94	0	0
6	H	2	Total 2	O 2	0	0
6	I	3	Total 3	O 3	0	0
6	J	3	Total 3	O 3	0	0
6	K	2	Total 2	O 2	0	0
6	L	3	Total 3	O 3	0	0
6	N	2	Total 2	O 2	0	0

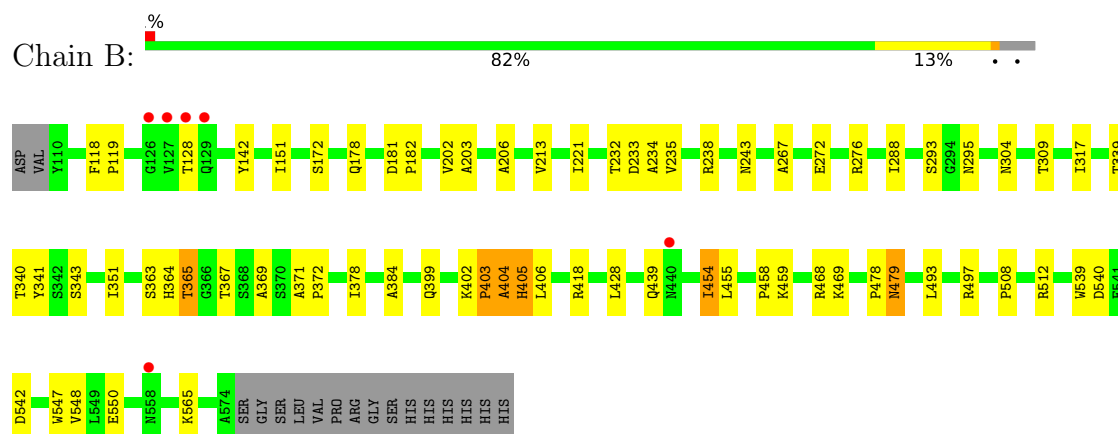
3 Residue-property plots [i](#)

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.

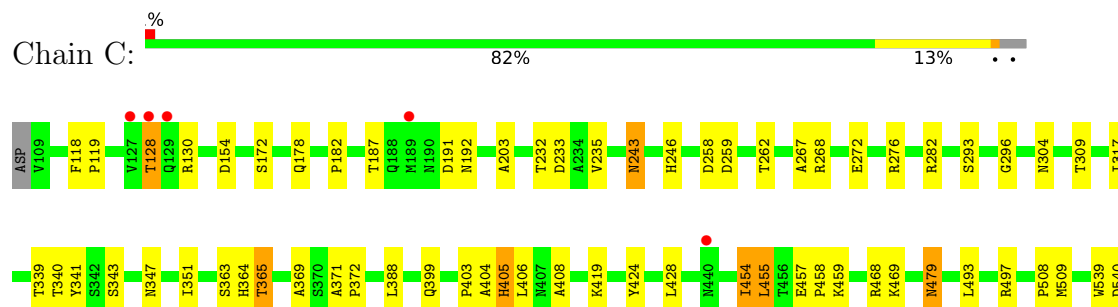
• Molecule 1: Furin

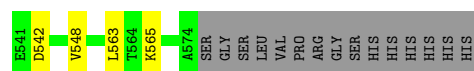


• Molecule 1: Furin

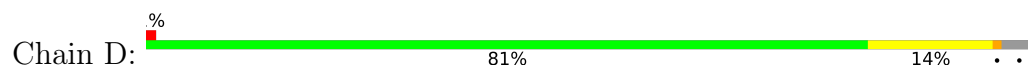


• Molecule 1: Furin

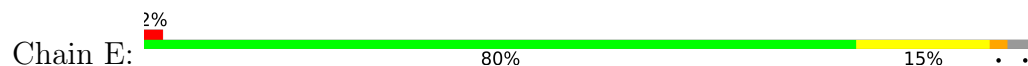




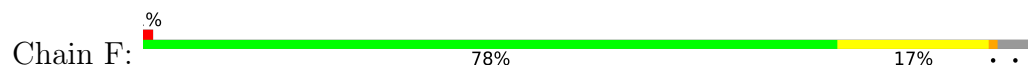
• Molecule 1: Furin



• Molecule 1: Furin



• Molecule 1: Furin



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

Chain H:  100%

There are no outlier residues recorded for this chain.

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

Chain I:  80% 20%



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

Chain J:  100%

There are no outlier residues recorded for this chain.

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

Chain K:  80% 20%



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

Chain L:  80% 20%



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

Chain N:  80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.62Å 152.61Å 168.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.5 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.218 0.193 , 0.218	Depositor DCC
R_{free} test set	5025 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.1	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	0.94	EDS
Total number of atoms	22341	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, HY1

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	0.44	0/3641	0.93	9/4964 (0.2%)
1	B	0.42	0/3634	0.94	11/4954 (0.2%)
1	C	0.43	0/3641	0.93	11/4964 (0.2%)
1	D	0.43	0/3634	0.93	9/4954 (0.2%)
1	E	0.42	0/3634	0.92	14/4954 (0.3%)
1	F	0.41	0/3634	0.93	10/4954 (0.2%)
2	H	0.26	0/28	1.01	0/35
2	I	0.29	0/28	1.08	0/35
2	J	0.30	0/28	1.04	0/35
2	K	0.23	0/28	0.99	0/35
2	L	0.27	0/28	1.09	0/35
2	N	0.27	0/28	1.10	0/35
All	All	0.43	0/21986	0.93	64/29954 (0.2%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	454	ILE	N-CA-C	8.38	119.24	111.45
1	B	454	ILE	N-CA-C	8.28	119.15	111.45
1	D	454	ILE	N-CA-C	8.27	119.14	111.45
1	F	454	ILE	N-CA-C	8.23	119.10	111.45
1	A	454	ILE	N-CA-C	8.12	119.01	111.45
1	B	243	ASN	CB-CA-C	-8.04	105.49	111.20
1	E	454	ILE	N-CA-C	7.82	118.72	111.45
1	F	243	ASN	CB-CA-C	-7.68	105.74	111.20
1	B	203	ALA	N-CA-C	7.57	120.07	110.61
1	E	203	ALA	N-CA-C	7.46	119.94	110.61
1	D	203	ALA	N-CA-C	7.43	119.90	110.61
1	A	203	ALA	N-CA-C	7.40	119.86	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	203	ALA	N-CA-C	7.20	119.61	110.61
1	A	243	ASN	CB-CA-C	-6.99	106.23	111.20
1	E	243	ASN	CB-CA-C	-6.73	106.42	111.20
1	C	203	ALA	N-CA-C	6.70	118.99	110.61
1	B	365	THR	N-CA-C	6.47	118.37	109.18
1	A	365	THR	N-CA-C	6.43	118.31	109.18
1	F	365	THR	N-CA-C	6.38	118.25	109.18
1	E	365	THR	N-CA-C	6.29	118.11	109.18
1	B	542	ASP	N-CA-C	-6.26	100.54	109.24
1	C	243	ASN	CB-CA-C	-6.26	106.76	111.20
1	C	542	ASP	N-CA-C	-6.17	100.66	109.24
1	C	365	THR	N-CA-C	5.98	117.68	109.18
1	E	542	ASP	N-CA-C	-5.92	101.01	109.24
1	D	365	THR	N-CA-C	5.91	117.57	109.18
1	D	455	LEU	N-CA-C	5.89	119.00	110.28
1	A	455	LEU	N-CA-C	5.85	118.94	110.28
1	D	542	ASP	N-CA-C	-5.83	101.14	109.24
1	E	455	LEU	N-CA-C	5.83	118.91	110.28
1	F	455	LEU	N-CA-C	5.66	118.66	110.28
1	C	455	LEU	N-CA-C	5.57	118.53	110.28
1	B	455	LEU	N-CA-C	5.53	118.46	110.28
1	F	304	ASN	N-CA-C	-5.52	106.55	113.28
1	A	542	ASP	N-CA-C	-5.48	101.63	109.24
1	F	317	ILE	N-CA-C	5.42	115.69	108.11
1	A	347	ASN	N-CA-C	-5.40	106.74	113.38
1	C	399	GLN	N-CA-C	5.38	118.06	111.82
1	D	243	ASN	CB-CA-C	-5.38	107.38	111.20
1	D	364	HIS	N-CA-C	-5.31	100.65	109.46
1	A	363	SER	N-CA-C	5.30	116.81	110.44
1	F	542	ASP	N-CA-C	-5.30	101.88	109.24
1	E	439	GLN	N-CA-C	5.30	117.05	111.28
1	B	363	SER	N-CA-C	5.29	116.79	110.44
1	C	304	ASN	N-CA-C	-5.28	106.84	113.28
1	E	399	GLN	N-CA-C	5.26	117.92	111.82
1	E	317	ILE	N-CA-C	5.24	115.44	108.11
1	E	410	ASP	N-CA-C	5.21	119.18	112.41
1	C	347	ASN	N-CA-C	-5.19	107.00	113.38
1	E	293	SER	N-CA-C	5.16	118.67	112.38
1	E	304	ASN	N-CA-C	-5.15	106.99	113.28
1	C	317	ILE	N-CA-C	5.14	115.31	108.11
1	F	347	ASN	N-CA-C	-5.14	107.05	113.38
1	D	317	ILE	N-CA-C	5.13	115.25	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	347	ASN	N-CA-C	-5.10	107.11	113.38
1	B	399	GLN	N-CA-C	5.10	117.73	111.82
1	A	364	HIS	N-CA-C	-5.08	101.03	109.46
1	D	537	HIS	N-CA-C	5.06	118.72	112.54
1	E	364	HIS	N-CA-C	-5.04	101.09	109.46
1	B	304	ASN	N-CA-C	-5.04	107.14	113.28
1	B	439	GLN	N-CA-C	5.04	116.77	111.28
1	F	456	THR	N-CA-C	-5.04	106.55	113.30
1	C	363	SER	N-CA-C	5.02	116.46	110.44
1	B	317	ILE	N-CA-C	5.01	115.07	107.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3559	0	3376	45	0
1	B	3552	0	3367	40	0
1	C	3559	0	3376	42	0
1	D	3552	0	3367	42	0
1	E	3552	0	3367	47	0
1	F	3552	0	3367	54	0
2	H	49	0	50	0	0
2	I	49	0	50	1	0
2	J	49	0	50	0	0
2	K	49	0	50	1	0
2	L	49	0	50	2	0
2	N	49	0	50	3	0
3	A	6	0	2	0	0
3	B	6	0	2	0	0
3	C	6	0	2	0	0
3	D	6	0	2	0	0
3	E	6	0	2	0	0
3	F	6	0	2	0	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	112	0	0	1	0
6	B	96	0	0	0	0
6	C	113	0	0	3	0
6	D	125	0	0	1	0
6	E	106	0	0	2	0
6	F	94	0	0	4	0
6	H	2	0	0	0	0
6	I	3	0	0	0	0
6	J	3	0	0	0	0
6	K	2	0	0	0	0
6	L	3	0	0	0	0
6	N	2	0	0	0	0
All	All	22341	0	20532	269	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 (269) 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:B:479:ASN:HD22	1:B:479:ASN:H	1.02	0.95
1:A:479:ASN:H	1:A:479:ASN:HD22	1.13	0.91
1:E:479:ASN:HD22	1:E:479:ASN:H	1.06	0.90
1:B:454:ILE:HD12	1:B:469:LYS:HG2	1.51	0.90
1:D:479:ASN:H	1:D:479:ASN:HD22	1.24	0.86
1:C:454:ILE:HD12	1:C:469:LYS:HG2	1.59	0.84
1:C:479:ASN:HD22	1:C:479:ASN:H	1.25	0.83
1:B:479:ASN:H	1:B:479:ASN:ND2	1.71	0.83
1:E:454:ILE:HD12	1:E:469:LYS:HG2	1.65	0.79
1:F:454:ILE:HD12	1:F:469:LYS:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:ASN:H	1:F:479:ASN:HD22	1.30	0.76
1:D:454:ILE:HD12	1:D:469:LYS:HG2	1.68	0.76
1:A:479:ASN:H	1:A:479:ASN:ND2	1.84	0.75
1:A:479:ASN:HD22	1:A:479:ASN:N	1.83	0.75
1:E:479:ASN:H	1:E:479:ASN:ND2	1.82	0.75
1:D:479:ASN:H	1:D:479:ASN:ND2	1.85	0.74
1:C:479:ASN:H	1:C:479:ASN:ND2	1.88	0.71
1:B:479:ASN:HD22	1:B:479:ASN:N	1.72	0.71
1:A:454:ILE:HD12	1:A:469:LYS:HG2	1.72	0.70
1:E:479:ASN:HD22	1:E:479:ASN:N	1.79	0.70
1:F:479:ASN:H	1:F:479:ASN:ND2	1.89	0.70
1:A:341:TYR:CE2	1:A:428:LEU:HD21	2.30	0.67
1:B:341:TYR:CE2	1:B:428:LEU:HD21	2.29	0.67
1:B:233:ASP:CG	1:B:267:ALA:HB3	2.21	0.66
1:C:479:ASN:HD22	1:C:479:ASN:N	1.88	0.63
1:E:341:TYR:CE2	1:E:428:LEU:HD21	2.33	0.63
1:C:493:LEU:C	1:C:493:LEU:HD12	2.24	0.62
1:C:268:ARG:HG3	6:C:810:HOH:O	1.99	0.61
1:C:341:TYR:CE2	1:C:428:LEU:HD21	2.35	0.61
1:F:479:ASN:HD22	1:F:479:ASN:N	1.92	0.61
1:C:172:SER:HB3	1:C:182:PRO:HG3	1.81	0.61
1:D:233:ASP:CG	1:D:267:ALA:HB3	2.26	0.61
1:F:333:CYS:HA	6:F:740:HOH:O	2.00	0.61
1:C:233:ASP:CG	1:C:267:ALA:HB3	2.26	0.60
1:E:493:LEU:C	1:E:493:LEU:HD12	2.26	0.60
1:C:468:ARG:HG2	1:C:548:VAL:HG22	1.85	0.59
1:A:493:LEU:C	1:A:493:LEU:HD12	2.27	0.59
1:C:458:PRO:O	1:C:459:LYS:HD2	2.02	0.59
1:A:293:SER:HA	1:A:309:THR:HG21	1.84	0.59
6:C:809:HOH:O	1:D:268:ARG:HG3	2.03	0.59
1:A:404:ALA:O	1:A:405:HIS:HB2	2.01	0.59
1:D:404:ALA:O	1:D:405:HIS:HB2	2.02	0.59
1:F:404:ALA:O	1:F:405:HIS:HB2	2.03	0.58
1:B:343:SER:OG	1:B:365:THR:HB	2.03	0.58
1:D:341:TYR:CE2	1:D:428:LEU:HD21	2.39	0.58
1:A:233:ASP:CG	1:A:267:ALA:HB3	2.28	0.58
1:B:404:ALA:O	1:B:405:HIS:HB2	2.03	0.58
1:C:404:ALA:O	1:C:405:HIS:HB2	2.02	0.58
1:B:458:PRO:O	1:B:459:LYS:HD2	2.04	0.57
1:F:341:TYR:CE2	1:F:428:LEU:HD21	2.40	0.57
1:D:371:ALA:HB3	1:D:372:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:SER:HA	1:F:309:THR:HG21	1.87	0.57
1:D:272:GLU:O	1:D:276:ARG:HG3	2.05	0.56
1:F:233:ASP:CG	1:F:267:ALA:HB3	2.30	0.56
1:B:512:ARG:HH12	1:B:550:GLU:CD	2.13	0.56
1:B:234:ALA:O	1:B:238:ARG:HG3	2.06	0.56
1:B:295:ASN:OD1	1:B:367:THR:HG22	2.05	0.56
1:F:351:ILE:HG13	1:F:369:ALA:HB1	1.88	0.56
1:B:172:SER:HB3	1:B:182:PRO:HG3	1.86	0.56
1:B:493:LEU:HD12	1:B:493:LEU:C	2.31	0.56
1:F:352:VAL:HG22	1:F:362:GLU:HG2	1.87	0.56
1:F:272:GLU:O	1:F:276:ARG:HG3	2.06	0.56
1:D:118:PHE:HB3	1:D:119:PRO:HD3	1.88	0.55
1:E:458:PRO:O	1:E:459:LYS:HD2	2.06	0.55
1:D:479:ASN:HD22	1:D:479:ASN:N	1.90	0.55
1:E:448:ARG:HD3	1:E:479:ASN:HA	1.88	0.55
1:A:118:PHE:HB3	1:A:119:PRO:HD3	1.88	0.55
1:D:458:PRO:O	1:D:459:LYS:HD2	2.08	0.54
1:B:293:SER:HA	1:B:309:THR:HG21	1.90	0.54
1:B:295:ASN:CG	1:B:367:THR:HG22	2.33	0.54
1:E:404:ALA:O	1:E:405:HIS:HB2	2.07	0.54
1:A:506:VAL:HG22	1:A:512:ARG:HG3	1.89	0.54
1:E:479:ASN:HB3	6:E:790:HOH:O	2.08	0.54
1:C:232:THR:OG1	1:C:235:VAL:HG23	2.08	0.54
1:D:206:ALA:HA	1:D:213:VAL:HG12	1.91	0.54
1:B:479:ASN:ND2	1:B:479:ASN:N	2.40	0.53
1:E:233:ASP:CG	1:E:267:ALA:HB3	2.32	0.53
1:F:458:PRO:O	1:F:459:LYS:HD2	2.08	0.53
1:F:172:SER:HB3	1:F:182:PRO:HG3	1.91	0.53
1:F:234:ALA:O	1:F:238:ARG:HG3	2.09	0.53
1:C:272:GLU:O	1:C:276:ARG:HG3	2.08	0.53
1:F:479:ASN:ND2	1:F:479:ASN:N	2.54	0.52
1:F:493:LEU:C	1:F:493:LEU:HD12	2.35	0.52
1:E:418:ARG:NH1	1:E:540:ASP:OD2	2.43	0.52
1:F:512:ARG:HD3	6:F:762:HOH:O	2.10	0.51
1:F:151:ILE:HG12	1:F:221:ILE:HD11	1.92	0.51
1:F:343:SER:OG	1:F:365:THR:HB	2.10	0.51
1:A:172:SER:HB3	1:A:182:PRO:HG3	1.93	0.51
1:B:272:GLU:O	1:B:276:ARG:HG3	2.10	0.51
1:A:295:ASN:OD1	1:A:367:THR:HG22	2.11	0.51
1:E:343:SER:OG	1:E:365:THR:HB	2.11	0.51
1:D:512:ARG:HH12	1:D:550:GLU:CD	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:LEU:HD12	1:D:493:LEU:C	2.35	0.50
1:D:553:ASN:ND2	1:D:559:ASN:HD22	2.09	0.50
1:A:207:ASN:HB3	1:C:419:LYS:HD3	1.93	0.50
1:A:399:GLN:HG2	1:A:418:ARG:HH22	1.77	0.50
1:B:118:PHE:HB3	1:B:119:PRO:HD3	1.93	0.50
1:A:371:ALA:HB3	1:A:372:PRO:HD3	1.94	0.50
1:E:454:ILE:CD1	1:E:469:LYS:HG2	2.40	0.50
1:C:351:ILE:HG13	1:C:369:ALA:HB1	1.93	0.49
1:C:479:ASN:ND2	1:C:479:ASN:N	2.52	0.49
1:D:172:SER:HB3	1:D:182:PRO:HG3	1.95	0.49
1:E:399:GLN:HG2	1:E:418:ARG:HH22	1.77	0.49
1:A:404:ALA:O	1:A:405:HIS:CB	2.61	0.49
1:F:341:TYR:CZ	1:F:428:LEU:HD21	2.47	0.49
1:A:539:TRP:O	1:A:540:ASP:HB2	2.12	0.49
1:E:295:ASN:CG	1:E:367:THR:HG22	2.37	0.49
1:D:295:ASN:OD1	1:D:367:THR:HG22	2.13	0.49
1:F:194:HIS:CB	2:N:4:ARG:HD3	2.42	0.49
1:F:295:ASN:OD1	1:F:367:THR:HG22	2.12	0.49
1:A:464:ARG:NH2	1:A:466:GLU:OE2	2.46	0.49
1:C:371:ALA:HB3	1:C:372:PRO:HD3	1.93	0.49
1:D:512:ARG:NH1	1:D:550:GLU:OE1	2.43	0.49
1:F:539:TRP:O	1:F:540:ASP:HB2	2.13	0.49
1:E:282:ARG:NH2	1:E:388:LEU:O	2.33	0.49
1:E:394:GLN:O	1:E:398:VAL:HG23	2.11	0.49
1:A:341:TYR:CZ	1:A:428:LEU:HD21	2.47	0.48
1:A:128:THR:O	1:A:130:ARG:HG2	2.14	0.48
1:E:233:ASP:OD2	1:E:269:LEU:HB2	2.13	0.48
1:F:288:ILE:HG21	1:F:378:ILE:HG21	1.95	0.48
1:A:343:SER:OG	1:A:365:THR:HB	2.13	0.48
1:D:333:CYS:HA	6:D:729:HOH:O	2.13	0.48
1:C:539:TRP:O	1:C:540:ASP:HB2	2.14	0.48
1:B:512:ARG:NH1	1:B:550:GLU:OE1	2.46	0.48
1:B:539:TRP:O	1:B:540:ASP:HB2	2.12	0.48
1:E:272:GLU:O	1:E:276:ARG:HG3	2.14	0.48
1:A:418:ARG:NH1	1:A:540:ASP:OD2	2.47	0.48
1:B:454:ILE:CD1	1:B:469:LYS:HG2	2.35	0.48
1:D:374:ALA:O	1:D:378:ILE:HG13	2.14	0.48
1:D:343:SER:OG	1:D:365:THR:HB	2.14	0.47
1:E:512:ARG:HH12	1:E:550:GLU:CD	2.22	0.47
1:A:141:GLY:HA3	1:C:509:MET:HE3	1.97	0.47
1:B:232:THR:OG1	1:B:235:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:ASN:ND2	1:E:479:ASN:N	2.49	0.47
1:E:539:TRP:O	1:E:540:ASP:HB2	2.14	0.47
1:C:154:ASP:OD2	1:C:192:ASN:HA	2.13	0.47
1:B:508:PRO:HD3	1:B:547:TRP:CE2	2.49	0.47
1:D:288:ILE:HG21	1:D:378:ILE:HG21	1.95	0.47
1:A:454:ILE:HG13	1:A:566:PHE:CE2	2.49	0.47
1:B:151:ILE:HG12	1:B:221:ILE:HD11	1.97	0.47
1:D:404:ALA:O	1:D:405:HIS:CB	2.63	0.47
1:E:232:THR:OG1	1:E:235:VAL:HG23	2.14	0.47
2:I:4:ARG:HG3	2:I:4:ARG:HH11	1.80	0.47
1:D:448:ARG:HD3	1:D:479:ASN:HA	1.97	0.47
1:C:404:ALA:O	1:C:405:HIS:CB	2.63	0.47
1:D:479:ASN:ND2	1:D:479:ASN:N	2.50	0.47
1:E:419:LYS:HD3	6:E:785:HOH:O	2.14	0.46
1:A:399:GLN:HG2	1:A:418:ARG:NH2	2.30	0.46
1:B:418:ARG:NH1	1:B:540:ASP:OD2	2.49	0.46
1:E:371:ALA:HB3	1:E:372:PRO:HD3	1.97	0.46
1:B:351:ILE:HG13	1:B:369:ALA:HB1	1.96	0.46
1:B:404:ALA:O	1:B:405:HIS:CB	2.63	0.46
1:A:458:PRO:O	1:A:459:LYS:HD2	2.15	0.46
1:C:118:PHE:N	1:C:119:PRO:CD	2.79	0.46
1:D:232:THR:OG1	1:D:235:VAL:HG23	2.16	0.46
1:F:468:ARG:HG2	1:F:548:VAL:HG22	1.97	0.46
1:B:233:ASP:OD1	1:B:267:ALA:HB3	2.15	0.46
1:A:207:ASN:CB	1:C:419:LYS:HD3	2.46	0.46
1:A:304:ASN:CG	1:A:333:CYS:HB2	2.41	0.46
1:B:371:ALA:HB3	1:B:372:PRO:HD3	1.98	0.46
1:C:455:LEU:HD11	1:C:563:LEU:HG	1.97	0.46
1:D:351:ILE:HG13	1:D:369:ALA:HB1	1.98	0.46
1:E:468:ARG:HG2	1:E:548:VAL:HG22	1.98	0.46
1:B:468:ARG:HG2	1:B:548:VAL:HG22	1.98	0.45
1:D:468:ARG:HG2	1:D:548:VAL:HG22	1.98	0.45
1:F:512:ARG:HH12	1:F:550:GLU:CD	2.24	0.45
1:C:293:SER:HA	1:C:309:THR:HG21	1.98	0.45
1:C:343:SER:OG	1:C:365:THR:HB	2.16	0.45
1:A:295:ASN:CG	1:A:367:THR:HG22	2.41	0.45
1:F:399:GLN:HG2	1:F:418:ARG:HH22	1.81	0.45
1:E:351:ILE:HG13	1:E:369:ALA:HB1	1.98	0.45
1:F:243:ASN:HB3	1:F:246:HIS:HB3	1.99	0.45
1:F:298:ARG:HD2	1:F:299:GLU:OE2	2.17	0.45
1:E:288:ILE:HG21	1:E:378:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:ASN:CG	1:F:367:THR:HG22	2.42	0.45
1:F:378:ILE:HG23	1:F:393:MET:HE3	1.99	0.45
1:B:288:ILE:HG21	1:B:378:ILE:HG21	1.99	0.45
1:C:457:GLU:HG3	1:C:459:LYS:HE3	1.99	0.45
1:D:295:ASN:CG	1:D:367:THR:HG22	2.42	0.45
1:D:539:TRP:O	1:D:540:ASP:HB2	2.17	0.45
1:F:404:ALA:O	1:F:405:HIS:CB	2.63	0.45
1:D:418:ARG:NH1	1:D:540:ASP:OD2	2.49	0.45
1:C:508:PRO:HD2	6:C:710:HOH:O	2.17	0.44
1:B:142:TYR:CE1	1:B:384:ALA:HA	2.53	0.44
1:F:118:PHE:N	1:F:119:PRO:CD	2.81	0.44
1:F:145:HIS:HB3	1:F:383:GLU:OE2	2.17	0.44
1:C:243:ASN:HB3	1:C:246:HIS:HB3	1.99	0.44
1:E:399:GLN:HG2	1:E:418:ARG:NH2	2.33	0.44
1:B:351:ILE:HB	1:B:364:HIS:HB3	1.99	0.44
1:D:143:THR:CB	1:D:218:ASN:HD22	2.31	0.44
1:F:339:THR:HG22	1:F:340:THR:N	2.32	0.44
1:C:128:THR:O	1:C:130:ARG:HG2	2.17	0.44
1:E:243:ASN:HB3	1:E:246:HIS:HB3	1.99	0.43
1:C:233:ASP:OD1	1:C:267:ALA:HB3	2.17	0.43
1:F:267:ALA:O	1:F:271:GLU:HG3	2.18	0.43
1:F:512:ARG:NH1	1:F:550:GLU:OE1	2.50	0.43
1:F:282:ARG:HD3	1:F:286:GLY:O	2.18	0.43
1:F:464:ARG:NH2	1:F:466:GLU:OE2	2.51	0.43
1:C:351:ILE:HB	1:C:364:HIS:HB3	1.99	0.43
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.85	0.43
1:E:118:PHE:N	1:E:119:PRO:CD	2.80	0.43
1:E:259:ASP:OD2	1:E:262:THR:HG23	2.17	0.43
1:B:339:THR:HG22	1:B:340:THR:N	2.33	0.43
1:C:282:ARG:NH2	1:C:388:LEU:O	2.39	0.43
1:A:150:SER:HB2	1:A:247:ILE:HD13	2.01	0.43
1:E:404:ALA:O	1:E:405:HIS:CB	2.67	0.43
1:F:117:LYS:HD3	1:F:120:GLN:OE1	2.19	0.43
2:N:4:ARG:HG3	2:N:4:ARG:HH11	1.84	0.43
1:A:333:CYS:HA	6:A:789:HOH:O	2.19	0.43
1:E:403:PRO:O	1:E:404:ALA:C	2.62	0.43
1:F:194:HIS:HB2	2:N:4:ARG:HD3	2.00	0.43
1:A:288:ILE:HG21	1:A:378:ILE:HG21	2.01	0.42
1:A:304:ASN:OD1	1:A:333:CYS:HB2	2.19	0.42
1:C:408:ALA:HB2	1:C:424:TYR:CE2	2.54	0.42
1:D:395:HIS:CD2	1:D:444:VAL:HG11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:HG22	1:B:372:PRO:O	2.20	0.42
1:E:339:THR:HG22	1:E:340:THR:N	2.34	0.42
1:B:181:ASP:C	1:B:181:ASP:OD1	2.60	0.42
1:C:341:TYR:CZ	1:C:428:LEU:HD21	2.54	0.42
1:A:208:ASN:O	1:A:210:VAL:HG23	2.20	0.42
1:C:458:PRO:C	1:C:459:LYS:HD2	2.45	0.42
1:D:508:PRO:HD3	1:D:547:TRP:CE2	2.55	0.42
1:F:371:ALA:HB3	1:F:372:PRO:HD3	2.01	0.42
1:A:206:ALA:HA	1:A:213:VAL:HG12	2.02	0.42
1:B:206:ALA:HA	1:B:213:VAL:HG12	2.02	0.42
1:D:154:ASP:OD2	1:D:192:ASN:HA	2.20	0.42
1:B:402:LYS:HA	1:B:403:PRO:HD3	1.91	0.42
1:E:194:HIS:HB2	2:L:4:ARG:HD3	2.01	0.42
1:E:374:ALA:O	1:E:378:ILE:HG13	2.19	0.42
1:F:508:PRO:HD3	1:F:547:TRP:CE2	2.54	0.42
1:F:118:PHE:HB3	1:F:119:PRO:HD3	2.02	0.42
1:F:315:LEU:HD22	1:F:378:ILE:HD11	2.02	0.42
1:A:259:ASP:OD2	1:A:262:THR:HG23	2.19	0.41
1:E:482:THR:OG1	1:E:574:ALA:HA	2.20	0.41
2:K:4:ARG:HG3	2:K:4:ARG:HH11	1.84	0.41
1:F:243:ASN:N	1:F:244:PRO:HD3	2.36	0.41
1:D:243:ASN:HB3	1:D:246:HIS:HB3	2.01	0.41
1:E:295:ASN:ND2	1:E:367:THR:HG22	2.35	0.41
1:F:457:GLU:HG3	1:F:459:LYS:HE3	2.02	0.41
1:A:351:ILE:HG13	1:A:369:ALA:HB1	2.02	0.41
1:A:512:ARG:NH2	1:A:550:GLU:OE2	2.40	0.41
1:C:259:ASP:OD2	1:C:262:THR:HG23	2.20	0.41
1:C:339:THR:HG22	1:C:340:THR:N	2.36	0.41
1:C:419:LYS:HE2	1:C:419:LYS:HB3	1.86	0.41
1:E:142:TYR:CE1	1:E:384:ALA:HA	2.55	0.41
1:A:468:ARG:HG2	1:A:548:VAL:HG22	2.02	0.41
1:E:160:HIS:CD2	1:E:358:GLN:HA	2.56	0.41
1:E:295:ASN:OD1	1:E:367:THR:HG22	2.20	0.41
1:A:306:ASP:OD1	1:A:306:ASP:C	2.64	0.41
1:D:304:ASN:CG	1:D:333:CYS:HB2	2.46	0.41
1:D:538:SER:HA	1:D:541:GLU:OE2	2.20	0.41
1:E:158:LYS:NZ	1:E:181:ASP:OD1	2.53	0.41
1:F:113:PRO:HB3	1:F:213:VAL:HG11	2.01	0.41
1:F:542:ASP:HB3	6:F:741:HOH:O	2.21	0.41
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.88	0.40
1:E:194:HIS:CB	2:L:4:ARG:HD3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:HB3	1:A:246:HIS:HB3	2.03	0.40
1:A:351:ILE:HB	1:A:364:HIS:HB3	2.02	0.40
1:C:258:ASP:HB3	1:C:296:GLY:CA	2.51	0.40
1:E:484:LEU:HD12	1:E:571:TYR:O	2.22	0.40
1:F:505:LEU:HB2	1:F:515:LEU:HD11	2.03	0.40
1:A:243:ASN:CG	1:B:478:PRO:HG2	2.47	0.40
1:D:353:THR:OG1	1:D:354:THR:N	2.54	0.40
1:F:484:LEU:HD12	1:F:571:TYR:O	2.21	0.40
1:C:187:THR:OG1	1:C:191:ASP:OD1	2.33	0.40
1:D:403:PRO:O	1:D:404:ALA:C	2.64	0.40
1:E:183:GLN:HA	1:E:184:PRO:HD3	1.96	0.40
1:F:268:ARG:HG3	6:F:787:HOH:O	2.21	0.40
1:F:382:LEU:HD23	1:F:382:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/482 (96%)	441 (95%)	20 (4%)	3 (1%)	21	44
1	B	463/482 (96%)	440 (95%)	19 (4%)	4 (1%)	14	35
1	C	464/482 (96%)	442 (95%)	19 (4%)	3 (1%)	21	44
1	D	463/482 (96%)	441 (95%)	19 (4%)	3 (1%)	21	44
1	E	463/482 (96%)	440 (95%)	19 (4%)	4 (1%)	14	35
1	F	463/482 (96%)	441 (95%)	19 (4%)	3 (1%)	21	44
2	H	2/5 (40%)	2 (100%)	0	0	100	100
2	I	2/5 (40%)	2 (100%)	0	0	100	100
2	J	2/5 (40%)	2 (100%)	0	0	100	100
2	K	2/5 (40%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	2/5 (40%)	2 (100%)	0	0	100	100
2	N	2/5 (40%)	2 (100%)	0	0	100	100
All	All	2792/2922 (96%)	2657 (95%)	115 (4%)	20 (1%)	18	41

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	THR
1	D	128	THR
1	E	128	THR
1	F	128	THR
1	A	128	THR
1	A	405	HIS
1	B	128	THR
1	B	405	HIS
1	C	405	HIS
1	D	405	HIS
1	E	405	HIS
1	F	405	HIS
1	B	404	ALA
1	E	404	ALA
1	B	403	PRO
1	E	403	PRO
1	F	403	PRO
1	A	403	PRO
1	D	403	PRO
1	C	403	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/390 (96%)	370 (98%)	6 (2%)	55	80
1	B	375/390 (96%)	370 (99%)	5 (1%)	61	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	376/390 (96%)	371 (99%)	5 (1%)	61	83
1	D	375/390 (96%)	370 (99%)	5 (1%)	61	83
1	E	375/390 (96%)	368 (98%)	7 (2%)	50	77
1	F	375/390 (96%)	369 (98%)	6 (2%)	55	80
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%)	2236 (98%)	34 (2%)	57	81

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ASP
1	A	178	GLN
1	A	406	LEU
1	A	479	ASN
1	A	497	ARG
1	A	565	LYS
1	B	178	GLN
1	B	406	LEU
1	B	479	ASN
1	B	497	ARG
1	B	565	LYS
1	C	178	GLN
1	C	406	LEU
1	C	479	ASN
1	C	497	ARG
1	C	565	LYS
1	D	178	GLN
1	D	406	LEU
1	D	479	ASN
1	D	497	ARG
1	D	565	LYS
1	E	178	GLN
1	E	182	PRO

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Mol	Chain	Res	Type
1	E	406	LEU
1	E	479	ASN
1	E	497	ARG
1	E	508	PRO
1	E	565	LYS
1	F	153	ASP
1	F	178	GLN
1	F	230	GLU
1	F	406	LEU
1	F	479	ASN
1	F	565	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	HIS
1	A	325	ASN
1	A	346	GLN
1	A	387	ASN
1	A	479	ASN
1	B	325	ASN
1	B	346	GLN
1	B	387	ASN
1	B	479	ASN
1	B	488	GLN
1	C	111	GLN
1	C	176	ASN
1	C	300	HIS
1	C	325	ASN
1	C	346	GLN
1	C	387	ASN
1	C	479	ASN
1	D	218	ASN
1	D	243	ASN
1	D	300	HIS
1	D	346	GLN
1	D	387	ASN
1	D	479	ASN
1	D	488	GLN
1	E	120	GLN
1	E	243	ASN
1	E	300	HIS

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Mol	Chain	Res	Type
1	E	346	GLN
1	E	387	ASN
1	E	479	ASN
1	E	488	GLN
1	F	243	ASN
1	F	300	HIS
1	F	325	ASN
1	F	346	GLN
1	F	358	GLN
1	F	387	ASN
1	F	479	ASN
1	F	488	GLN
1	F	537	HIS

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 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	E	602	-	2,2,2	0.65	0	1,1,1	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FMT	B	602	-	2,2,2	0.63	0	1,1,1	0.05	0
3	FMT	C	601	-	2,2,2	0.69	0	1,1,1	0.02	0
3	FMT	B	601	-	2,2,2	0.69	0	1,1,1	0.00	0
3	FMT	F	601	-	2,2,2	0.67	0	1,1,1	0.01	0
3	FMT	E	601	-	2,2,2	0.63	0	1,1,1	0.07	0
3	FMT	F	602	-	2,2,2	0.63	0	1,1,1	0.06	0
3	FMT	C	602	-	2,2,2	0.65	0	1,1,1	0.05	0
3	FMT	A	601	-	2,2,2	0.67	0	1,1,1	0.01	0
3	FMT	D	601	-	2,2,2	0.65	0	1,1,1	0.02	0
3	FMT	A	602	-	2,2,2	0.64	0	1,1,1	0.05	0
3	FMT	D	602	-	2,2,2	0.61	0	1,1,1	0.06	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.54	5 (1%) 78 76	11, 21, 34, 45	13 (2%)
1	B	465/482 (96%)	-0.51	6 (1%) 75 73	12, 22, 35, 52	15 (3%)
1	C	466/482 (96%)	-0.57	5 (1%) 78 76	10, 20, 33, 47	14 (3%)
1	D	465/482 (96%)	-0.49	7 (1%) 72 70	12, 22, 35, 51	18 (3%)
1	E	465/482 (96%)	-0.46	9 (1%) 66 63	10, 22, 36, 56	13 (2%)
1	F	465/482 (96%)	-0.44	7 (1%) 72 70	13, 24, 37, 53	19 (4%)
2	H	3/5 (60%)	-0.78	0 100 100	16, 16, 20, 22	0
2	I	3/5 (60%)	-0.92	0 100 100	19, 19, 24, 26	0
2	J	3/5 (60%)	-1.01	0 100 100	18, 18, 20, 24	0
2	K	3/5 (60%)	-1.11	0 100 100	15, 15, 15, 21	0
2	L	3/5 (60%)	-0.82	0 100 100	20, 20, 22, 25	0
2	N	3/5 (60%)	-0.67	0 100 100	20, 20, 23, 26	0
All	All	2810/2922 (96%)	-0.50	39 (1%) 73 72	10, 22, 35, 56	92 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	127	VAL	5.5
1	F	128	THR	4.7
1	C	128	THR	4.4
1	F	127	VAL	4.2
1	D	128	THR	4.2
1	E	129	GLN	4.2
1	B	128	THR	4.0
1	E	128	THR	4.0
1	E	110	TYR	3.8
1	D	129	GLN	3.6
1	A	127	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	128	THR	3.5
1	F	129	GLN	3.5
1	A	129	GLN	3.4
1	D	127	VAL	3.4
1	C	129	GLN	3.4
1	B	127	VAL	3.3
1	F	440	ASN	3.2
1	E	126	GLY	2.9
1	C	440	ASN	2.9
1	B	129	GLN	2.8
1	D	358	GLN	2.7
1	C	127	VAL	2.6
1	A	440	ASN	2.6
1	E	405	HIS	2.5
1	B	558	ASN	2.3
1	D	126	GLY	2.3
1	F	558	ASN	2.2
1	F	126	GLY	2.2
1	B	126	GLY	2.2
1	D	130	ARG	2.2
1	B	440	ASN	2.2
1	F	110	TYR	2.2
1	E	440	ASN	2.1
1	E	125	SER	2.1
1	A	130	ARG	2.1
1	C	189	MET	2.1
1	D	440	ASN	2.0
1	E	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	0.85	0.14	29,29,32,34	0
3	FMT	C	601	3/3	0.87	0.13	33,33,34,37	0
3	FMT	A	601	3/3	0.91	0.10	26,26,28,31	0
3	FMT	F	601	3/3	0.91	0.11	32,32,36,37	0
3	FMT	D	601	3/3	0.93	0.09	28,28,29,30	0
3	FMT	E	601	3/3	0.95	0.10	25,25,26,27	0
3	FMT	C	602	3/3	0.96	0.08	34,34,35,35	0
4	CA	B	605	1/1	0.96	0.07	42,42,42,42	0
3	FMT	F	602	3/3	0.97	0.06	19,19,21,23	0
3	FMT	D	602	3/3	0.97	0.06	22,22,26,30	0
4	CA	C	605	1/1	0.97	0.03	33,33,33,33	0
4	CA	D	605	1/1	0.97	0.04	32,32,32,32	0
4	CA	E	605	1/1	0.97	0.04	35,35,35,35	0
3	FMT	E	602	3/3	0.98	0.06	22,22,22,25	0
3	FMT	B	602	3/3	0.98	0.07	32,32,33,33	0
3	FMT	A	602	3/3	0.98	0.07	33,33,33,33	0
4	CA	A	605	1/1	0.98	0.03	35,35,35,35	0
5	NA	D	606	1/1	0.98	0.04	21,21,21,21	0
4	CA	B	604	1/1	0.99	0.03	18,18,18,18	0
4	CA	D	603	1/1	0.99	0.02	30,30,30,30	0
4	CA	B	603	1/1	0.99	0.04	32,32,32,32	0
4	CA	E	603	1/1	0.99	0.02	28,28,28,28	0
4	CA	E	604	1/1	0.99	0.02	17,17,17,17	0
4	CA	C	603	1/1	0.99	0.01	18,18,18,18	0
4	CA	F	603	1/1	0.99	0.02	29,29,29,29	0
4	CA	F	604	1/1	0.99	0.03	17,17,17,17	0
4	CA	F	605	1/1	0.99	0.03	35,35,35,35	0
5	NA	A	606	1/1	0.99	0.02	11,11,11,11	0
5	NA	B	606	1/1	0.99	0.03	20,20,20,20	0
5	NA	C	606	1/1	0.99	0.03	21,21,21,21	0
4	CA	C	604	1/1	0.99	0.01	20,20,20,20	0
5	NA	E	606	1/1	0.99	0.03	17,17,17,17	0
5	NA	F	606	1/1	0.99	0.04	25,25,25,25	0
4	CA	A	604	1/1	1.00	0.01	15,15,15,15	0
4	CA	D	604	1/1	1.00	0.01	14,14,14,14	0
4	CA	A	603	1/1	1.00	0.02	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.