



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:19 PM UTC

PDB ID : 4IOF / pdb_00004iof
Title : Crystal structure analysis of Fab-bound human Insulin Degrading Enzyme (IDE)
Authors : McCord, L.A.; Liang, W.G.; Hoey, R.; Dowdell, E.; Koide, A.; Koide, S.; Tang, W.J.
Deposited on : 2013-01-07
Resolution : 3.35 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
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

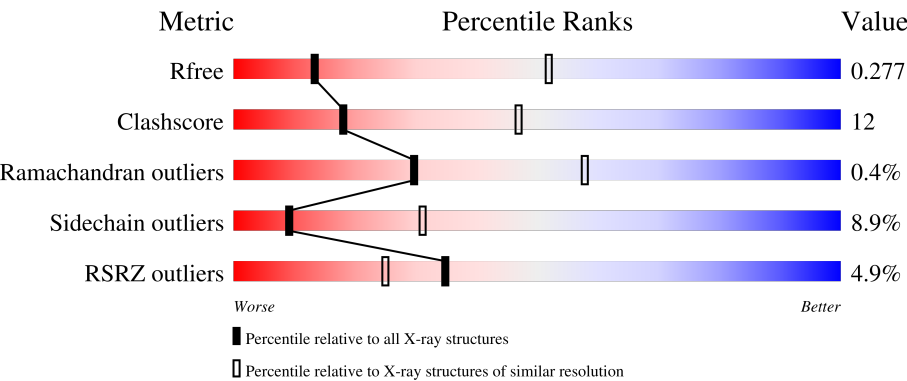
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	990	4% 73% 19% 6%
1	B	990	4% 59% 23% 13%
2	C	263	3% 44% 33% 5% 18%
2	E	263	5% 40% 36% 20%
3	D	239	5% 46% 30% 7% 17%

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Mol	Chain	Length	Quality of chain
3	F	239	4%41%35%5%18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20939 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	932	Total	C	N	O	S	0	0	0
			7622	4911	1274	1415	22			
1	B	861	Total	C	N	O	S	0	0	0
			7040	4550	1173	1296	21			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	conflict	UNP P14735
A	171	SER	CYS	conflict	UNP P14735
A	178	ALA	CYS	conflict	UNP P14735
A	257	VAL	CYS	conflict	UNP P14735
A	414	LEU	CYS	conflict	UNP P14735
A	573	ASN	CYS	conflict	UNP P14735
A	590	SER	CYS	conflict	UNP P14735
A	789	SER	CYS	conflict	UNP P14735
A	812	ALA	CYS	conflict	UNP P14735
A	819	ALA	CYS	conflict	UNP P14735
A	904	SER	CYS	conflict	UNP P14735
A	966	ASN	CYS	conflict	UNP P14735
A	974	ALA	CYS	conflict	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	conflict	UNP P14735
B	171	SER	CYS	conflict	UNP P14735
B	178	ALA	CYS	conflict	UNP P14735
B	257	VAL	CYS	conflict	UNP P14735
B	414	LEU	CYS	conflict	UNP P14735
B	573	ASN	CYS	conflict	UNP P14735
B	590	SER	CYS	conflict	UNP P14735
B	789	SER	CYS	conflict	UNP P14735
B	812	ALA	CYS	conflict	UNP P14735
B	819	ALA	CYS	conflict	UNP P14735
B	904	SER	CYS	conflict	UNP P14735
B	966	ASN	CYS	conflict	UNP P14735
B	974	ALA	CYS	conflict	UNP P14735

- Molecule 2 is a protein called Fab-bound IDE, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	216	Total	C	N	O	S	0	0	0
			1637	1043	268	319	7			
2	E	211	Total	C	N	O	S	0	0	0
			1602	1023	263	309	7			

- Molecule 3 is a protein called Fab-bound IDE, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	199	Total	C	N	O	S	0	0	0
			1528	962	255	306	5			
3	F	197	Total	C	N	O	S	0	0	0
			1508	947	250	306	5			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0

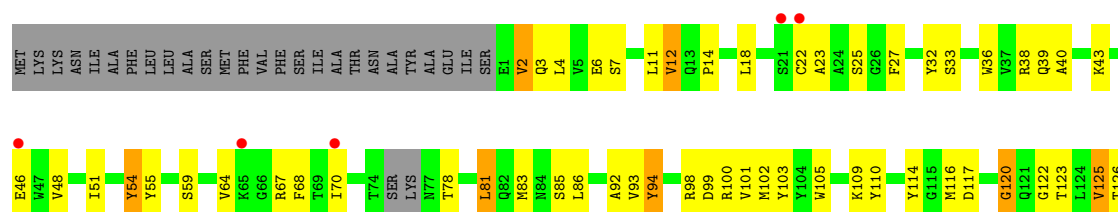
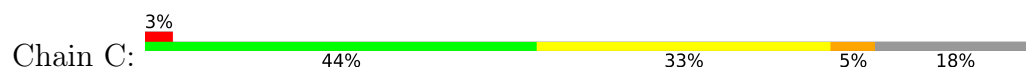
- Molecule 5 is water.

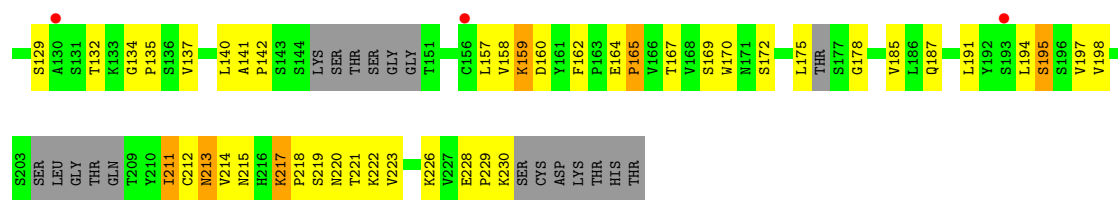
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	O 1	0	0

- Molecule 1: Insulin-degrading enzyme

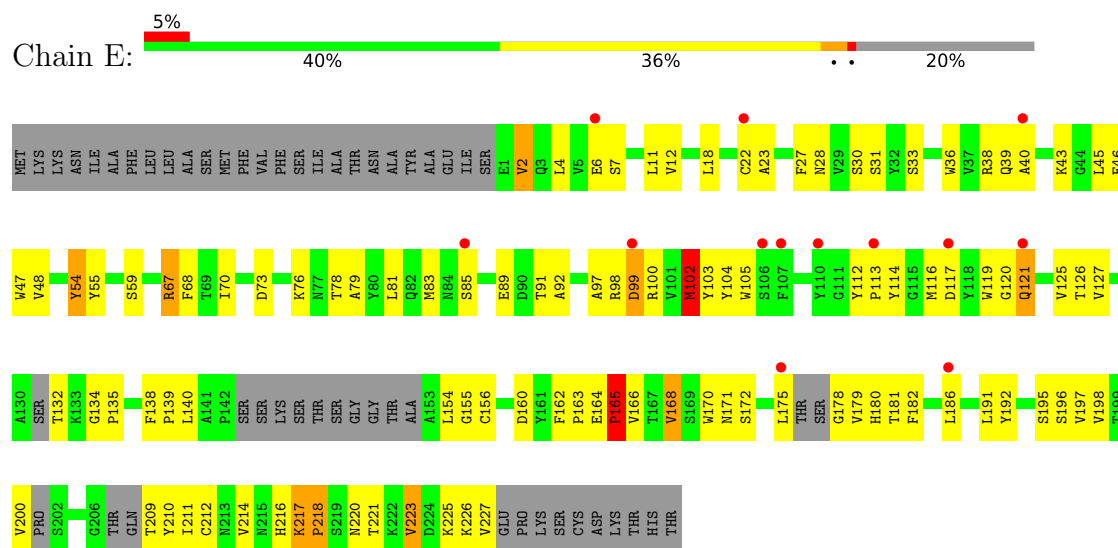


- Molecule 2: Fab-bound IDE, heavy chain

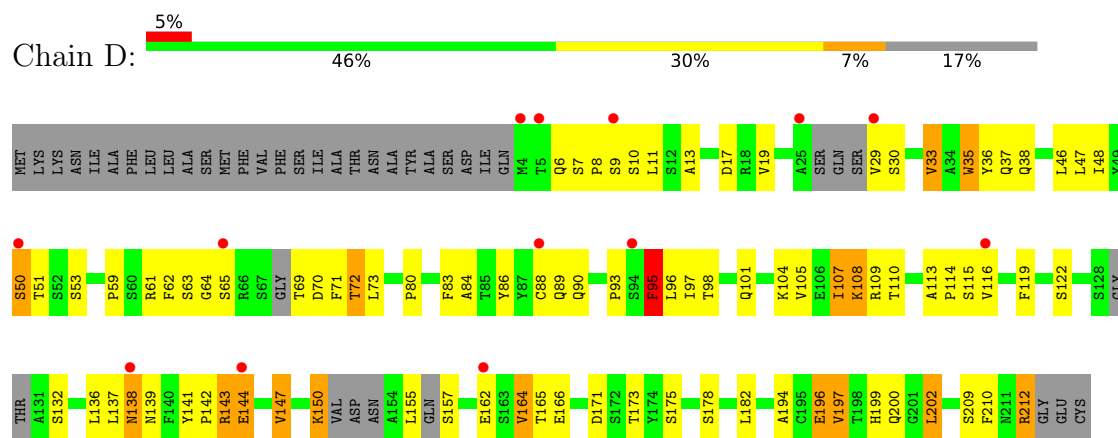




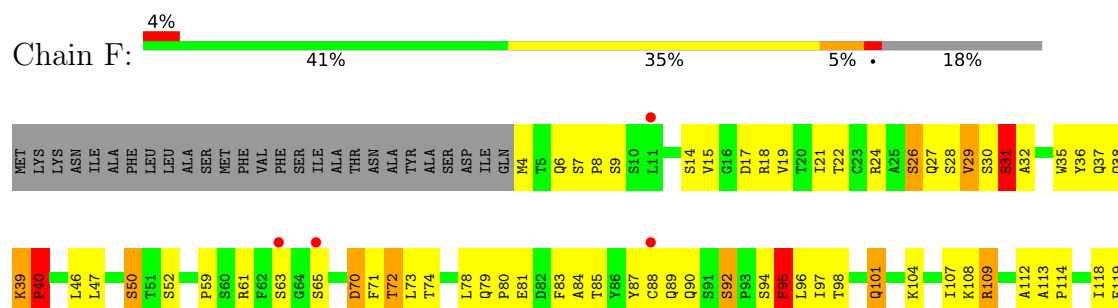
• Molecule 2: Fab-bound IDE, heavy chain

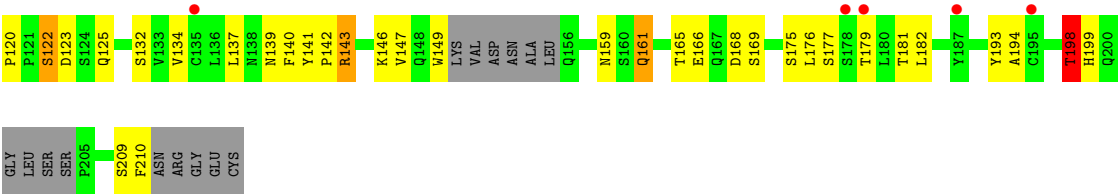


• Molecule 3: Fab-bound IDE, light chain



• Molecule 3: Fab-bound IDE, light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.95Å 131.66Å 377.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 3.35 49.85 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.85-3.35) 95.0 (49.85-3.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.232 , 0.280 0.235 , 0.277	Depositor DCC
R_{free} test set	2012 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	20939	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: ZN

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	0.42	0/7803	1.01	22/10549 (0.2%)
1	B	0.45	0/7206	1.09	50/9733 (0.5%)
2	C	0.44	0/1679	1.31	23/2285 (1.0%)
2	E	0.59	0/1641	1.30	17/2229 (0.8%)
3	D	0.43	0/1557	1.23	16/2106 (0.8%)
3	F	0.55	0/1540	1.36	17/2088 (0.8%)
All	All	0.46	0/21426	1.13	145/28990 (0.5%)

There are no bond length outliers.

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ASN	CB-CA-C	-18.67	79.86	111.23
2	E	220	ASN	CB-CA-C	-14.57	91.81	111.63
3	F	29	VAL	CB-CA-C	-13.38	89.35	111.29
2	E	114	TYR	N-CA-C	-10.11	95.56	110.52
3	F	101	GLN	N-CA-C	-10.04	94.90	109.96
3	D	50	SER	N-CA-C	-9.72	94.84	110.20
3	F	50	SER	N-CA-C	-9.49	95.21	110.20
1	B	451	THR	N-CA-C	-9.23	102.15	113.97
1	A	51	GLY	N-CA-C	-9.19	91.40	113.18
1	B	148	ASN	N-CA-C	9.16	124.24	108.76
3	F	92	SER	CA-C-N	-9.05	108.52	119.84
3	F	92	SER	C-N-CA	-9.05	108.52	119.84
2	E	102	MET	N-CA-C	8.98	121.00	111.03
1	B	94	ILE	N-CA-C	8.86	121.56	108.45
1	B	656	GLU	N-CA-C	8.64	120.31	111.07
1	B	102	ASN	N-CA-C	8.23	123.57	111.96
1	B	171	SER	C-N-CD	-8.13	91.66	125.00
3	F	31	SER	N-CA-C	-7.81	94.17	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	30	SER	N-CA-C	-7.71	98.06	109.62
2	C	134	GLY	CA-C-N	-7.65	110.27	119.84
2	C	134	GLY	C-N-CA	-7.65	110.27	119.84
2	C	120	GLY	N-CA-C	-7.60	99.52	112.51
2	C	217	LYS	CA-C-N	-7.44	110.79	119.05
2	C	217	LYS	C-N-CA	-7.44	110.79	119.05
2	C	219	SER	N-CA-C	-7.31	98.40	110.17
1	B	118	THR	N-CA-C	-7.28	99.18	110.17
1	B	126	GLU	N-CA-C	-7.25	103.69	112.54
3	D	63	SER	CA-C-N	-7.24	115.78	122.80
3	D	63	SER	C-N-CA	-7.24	115.78	122.80
3	D	64	GLY	N-CA-C	-7.22	97.86	110.71
1	A	280	ASN	CA-C-N	-7.17	112.49	123.17
1	A	280	ASN	C-N-CA	-7.17	112.49	123.17
3	D	200	GLN	N-CA-C	7.07	119.84	111.71
1	B	962	GLU	N-CA-C	7.05	121.11	112.23
1	B	99	ASP	N-CA-C	-6.96	101.59	109.60
3	F	137	LEU	N-CA-C	-6.92	98.44	109.59
2	E	114	TYR	CA-C-N	-6.85	114.55	122.83
2	E	114	TYR	C-N-CA	-6.85	114.55	122.83
2	E	120	GLY	N-CA-C	-6.82	103.39	112.81
2	E	134	GLY	CA-C-N	-6.79	111.35	119.84
2	E	134	GLY	C-N-CA	-6.79	111.35	119.84
1	B	825	THR	N-CA-C	6.76	118.31	111.07
1	A	656	GLU	N-CA-C	6.70	118.24	111.07
3	D	166	GLU	N-CA-C	-6.70	100.60	110.52
1	B	147	THR	N-CA-C	-6.66	98.98	109.50
1	B	93	HIS	CA-C-N	6.61	132.23	122.71
1	B	93	HIS	C-N-CA	6.61	132.23	122.71
1	B	86	SER	N-CA-C	-6.59	99.47	109.95
2	E	179	VAL	N-CA-C	6.56	117.28	107.51
3	F	95	PHE	N-CA-C	6.55	120.44	111.39
3	D	9	SER	N-CA-C	-6.49	103.33	111.11
1	B	329	ASN	CA-C-N	6.48	126.25	119.05
1	B	329	ASN	C-N-CA	6.48	126.25	119.05
3	F	72	THR	N-CA-C	6.41	119.15	108.13
1	A	279	GLU	CB-CA-C	-6.41	98.56	109.51
3	F	39	LYS	CA-C-N	6.37	127.81	119.84
3	F	39	LYS	C-N-CA	6.37	127.81	119.84
1	B	94	ILE	N-CA-CB	-6.37	101.00	111.45
2	C	228	GLU	CA-C-N	6.32	126.33	119.89
2	C	228	GLU	C-N-CA	6.32	126.33	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	96	LEU	N-CA-CB	-6.29	100.56	110.69
1	B	855	PRO	CA-C-N	6.26	126.46	119.32
1	B	855	PRO	C-N-CA	6.26	126.46	119.32
1	A	349	GLU	N-CA-C	6.26	117.77	111.07
3	D	95	PHE	N-CA-C	6.07	119.77	111.39
3	F	96	LEU	N-CA-CB	-6.03	100.98	110.69
3	D	197	VAL	N-CA-C	6.03	116.54	107.80
1	B	114	LEU	CB-CA-C	-6.02	98.59	110.27
1	B	114	LEU	N-CA-C	6.02	120.35	113.19
3	D	72	THR	N-CA-C	6.00	118.45	108.13
1	A	179	LYS	N-CA-C	5.99	117.48	111.07
2	C	220	ASN	N-CA-C	-5.99	99.44	108.96
1	A	521	LYS	N-CA-C	-5.96	105.97	113.18
3	D	105	VAL	CA-C-N	5.95	132.75	122.64
3	D	105	VAL	C-N-CA	5.95	132.75	122.64
1	B	986	LEU	CA-C-N	-5.91	114.54	120.21
1	B	986	LEU	C-N-CA	-5.91	114.54	120.21
3	F	139	ASN	CB-CA-C	-5.91	102.84	111.23
1	B	87	SER	N-CA-C	5.89	118.13	109.24
1	A	557	SER	N-CA-C	5.89	118.09	108.55
1	B	282	ASN	N-CA-C	5.89	119.15	109.85
2	E	218	PRO	N-CA-C	-5.88	105.05	113.47
3	D	93	PRO	CB-CA-C	5.87	121.25	111.56
2	C	12	VAL	N-CA-C	5.86	116.31	108.11
1	A	868	ILE	N-CA-C	5.85	116.03	110.42
2	E	168	VAL	CA-C-N	-5.85	113.63	122.81
2	E	168	VAL	C-N-CA	-5.85	113.63	122.81
2	C	219	SER	CA-C-N	-5.76	114.52	122.30
2	C	219	SER	C-N-CA	-5.76	114.52	122.30
3	F	71	PHE	N-CA-C	-5.76	100.50	109.72
3	D	210	PHE	N-CA-C	-5.75	100.56	109.24
1	B	280	ASN	N-CA-C	5.72	118.05	108.73
2	E	220	ASN	N-CA-C	5.71	119.56	111.92
1	B	868	ILE	N-CA-C	5.68	115.87	110.42
1	B	439	GLY	N-CA-C	-5.67	99.75	113.18
1	B	116	LEU	N-CA-C	5.66	116.53	108.54
3	D	35	TRP	N-CA-C	5.66	118.63	109.40
1	B	557	SER	N-CA-C	5.62	117.66	108.55
2	C	94	TYR	CA-C-N	5.59	132.15	122.64
2	C	94	TYR	C-N-CA	5.59	132.15	122.64
1	B	580	SER	CA-C-N	5.57	125.41	119.28
1	B	580	SER	C-N-CA	5.57	125.41	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	524	LEU	CA-C-N	-5.55	114.88	120.21
1	B	524	LEU	C-N-CA	-5.55	114.88	120.21
2	C	48	VAL	CB-CA-C	-5.54	107.00	111.71
1	A	524	LEU	CA-C-N	-5.53	114.90	120.21
1	A	524	LEU	C-N-CA	-5.53	114.90	120.21
1	B	921	ASP	N-CA-C	5.48	117.25	111.28
1	B	241	LEU	CA-C-N	5.47	127.61	120.28
1	B	241	LEU	C-N-CA	5.47	127.61	120.28
1	A	305	VAL	N-CA-C	5.47	113.28	107.76
1	B	95	GLY	N-CA-C	5.46	126.13	113.18
1	B	100	PRO	CA-C-N	5.44	126.59	120.66
1	B	100	PRO	C-N-CA	5.44	126.59	120.66
2	C	116	MET	N-CA-C	-5.44	98.33	108.02
1	A	116	LEU	N-CA-C	5.44	118.72	112.57
1	B	93	HIS	CB-CA-C	-5.39	103.93	111.80
2	C	114	TYR	N-CA-C	-5.37	103.30	110.55
1	B	118	THR	CB-CA-C	-5.31	100.98	111.60
2	E	112	TYR	CA-C-N	-5.29	113.23	119.84
2	E	112	TYR	C-N-CA	-5.29	113.23	119.84
1	A	197	ASP	N-CA-C	5.28	117.03	111.28
1	B	420	VAL	N-CA-C	-5.25	105.42	110.72
1	A	855	PRO	CA-C-N	5.24	124.69	119.24
1	A	855	PRO	C-N-CA	5.24	124.69	119.24
1	A	99	ASP	CA-C-N	5.23	125.77	120.38
1	A	99	ASP	C-N-CA	5.23	125.77	120.38
2	C	48	VAL	N-CA-C	5.22	116.39	111.48
3	F	139	ASN	N-CA-C	5.18	117.44	107.44
2	E	217	LYS	N-CA-C	5.17	121.23	109.81
2	E	48	VAL	CB-CA-C	-5.14	107.34	111.71
2	C	219	SER	CB-CA-C	5.14	118.19	109.50
1	A	993	GLN	N-CA-C	-5.13	107.15	113.41
2	C	134	GLY	N-CA-C	-5.13	101.88	112.34
1	A	347	LEU	N-CA-C	-5.12	105.70	111.28
1	B	637	LYS	N-CA-C	-5.12	105.10	113.19
2	C	169	SER	N-CA-C	5.11	117.90	109.72
1	B	441	LEU	N-CA-C	-5.11	106.31	112.54
1	B	170	LEU	N-CA-C	-5.11	106.19	112.72
1	B	349	GLU	N-CA-C	5.10	116.52	111.07
2	C	218	PRO	N-CA-C	-5.08	106.47	113.53
1	B	437	ILE	CB-CA-C	-5.07	104.29	111.28
2	C	93	VAL	N-CA-C	5.06	115.37	107.99
1	B	826	LYS	N-CA-C	5.04	117.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	198	THR	N-CA-C	-5.01	102.65	110.42

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	7622	0	7588	108	0
1	B	7040	0	7032	166	0
2	C	1637	0	1577	58	0
2	E	1602	0	1548	79	0
3	D	1528	0	1501	52	0
3	F	1508	0	1472	64	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	20939	0	20718	506	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 12.

All (506) 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)
2:E:216:HIS:ND1	2:E:218:PRO:HD2	1.68	1.09
3:F:27:GLN:HG3	3:F:28:SER:H	1.17	1.08
1:B:118:THR:HG21	1:B:167:GLN:CB	1.87	1.04
1:B:118:THR:HG21	1:B:167:GLN:HB3	1.03	1.00
1:B:118:THR:CG2	1:B:167:GLN:HB3	1.97	0.94
1:B:173:LEU:HD13	1:B:174:PHE:C	1.91	0.94
3:D:115:SER:HB2	3:D:138:ASN:CB	1.99	0.93
1:B:114:LEU:O	1:B:114:LEU:HG	1.71	0.87
3:D:115:SER:HB2	3:D:138:ASN:HB2	1.56	0.85
1:A:765:ARG:HH11	1:A:765:ARG:HG2	1.40	0.84
2:C:40:ALA:HB3	2:C:43:LYS:HB2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:137:LEU:HD21	3:D:197:VAL:HG11	1.62	0.82
2:E:67:ARG:HG3	2:E:85:SER:HB2	1.60	0.82
1:B:768:GLU:HB3	1:B:843:ILE:HD13	1.62	0.82
1:B:519:ASN:ND2	1:B:521:LYS:H	1.79	0.81
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.61	0.80
2:E:216:HIS:CE1	2:E:218:PRO:HD2	2.17	0.80
3:F:143:ARG:HH11	3:F:143:ARG:HB3	1.47	0.79
1:B:519:ASN:HD22	1:B:519:ASN:C	1.90	0.79
1:B:528:ASN:HD21	1:B:530:PHE:HB2	1.48	0.78
1:A:771:LEU:H	1:A:796:GLN:HE22	1.32	0.77
3:F:27:GLN:HG3	3:F:28:SER:N	1.93	0.76
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.50	0.76
1:A:573:ASN:ND2	1:A:632:LYS:HB3	2.01	0.75
1:B:573:ASN:ND2	1:B:632:LYS:HB3	2.02	0.75
2:E:99:ASP:N	2:E:99:ASP:OD1	2.19	0.75
1:A:423:ARG:HH11	1:A:423:ARG:CG	1.99	0.75
1:B:557:SER:HB3	1:B:742:MET:HE3	1.69	0.74
1:B:519:ASN:HD22	1:B:520:GLY:N	1.86	0.74
1:A:460:ARG:NH2	2:C:102:MET:O	2.20	0.74
1:B:118:THR:HG23	1:B:171:SER:O	1.88	0.74
1:A:620:LEU:HD13	1:A:629:LEU:HD13	1.71	0.73
3:F:165:THR:HG22	3:F:175:SER:H	1.53	0.73
1:B:92:VAL:HG12	1:B:92:VAL:O	1.88	0.73
1:B:123:LYS:HE2	1:B:126:GLU:HB2	1.71	0.73
2:E:23:ALA:HA	2:E:78:THR:HG23	1.69	0.73
1:B:115:PHE:CD1	1:B:168:PHE:CE2	2.76	0.73
2:E:39:GLN:O	2:E:92:ALA:HB1	1.90	0.72
1:B:118:THR:HG22	1:B:119:LYS:H	1.55	0.72
3:F:4:MET:HG3	3:F:26:SER:OG	1.89	0.71
3:D:13:ALA:HA	3:D:108:LYS:HZ2	1.56	0.71
1:B:797:THR:HG23	1:B:943:MET:HE2	1.71	0.71
1:B:572:ALA:HB3	1:B:638:GLN:HE22	1.55	0.71
1:B:388:GLU:OE2	1:B:512:LYS:HE2	1.91	0.71
1:B:893:ARG:NH2	1:B:921:ASP:OD1	2.25	0.70
1:B:255:ALA:HB1	1:B:441:LEU:HD12	1.74	0.70
1:B:809:GLU:OE2	1:B:839:ARG:NH2	2.23	0.70
3:D:89:GLN:HG2	3:D:90:GLN:N	2.07	0.70
2:E:135:PRO:HD3	2:E:216:HIS:HD2	1.57	0.69
2:C:39:GLN:O	2:C:92:ALA:HB1	1.92	0.69
3:F:89:GLN:HG2	3:F:90:GLN:N	2.06	0.69
1:A:229:ARG:NE	1:A:233:GLU:OE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ARG:HG2	1:A:765:ARG:NH1	2.05	0.69
1:B:173:LEU:O	1:B:173:LEU:HD22	1.92	0.69
1:B:48:LYS:HG2	1:B:49:ARG:H	1.57	0.69
3:F:59:PRO:HB3	3:F:61:ARG:NH1	2.08	0.69
1:B:528:ASN:ND2	1:B:530:PHE:H	1.91	0.68
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.75	0.68
1:A:935:ASP:HA	1:A:938:LYS:HE2	1.74	0.68
1:B:173:LEU:HD22	1:B:173:LEU:C	2.18	0.68
2:C:23:ALA:HA	2:C:78:THR:HG23	1.74	0.68
3:F:39:LYS:HD3	3:F:84:ALA:HB2	1.75	0.68
2:E:216:HIS:ND1	2:E:218:PRO:CD	2.54	0.68
1:A:465:GLU:HG2	2:C:105:TRP:HZ3	1.58	0.68
1:B:519:ASN:HD22	1:B:521:LYS:H	1.39	0.67
3:F:134:VAL:HG22	3:F:179:THR:HG23	1.77	0.67
3:F:159:ASN:ND2	3:F:181:THR:O	2.26	0.67
1:B:118:THR:HG22	1:B:119:LYS:N	2.09	0.67
2:C:67:ARG:C	2:C:68:PHE:HD1	2.01	0.67
2:E:67:ARG:HB3	2:E:68:PHE:HD1	1.60	0.67
1:B:559:LEU:HB2	1:B:742:MET:HE2	1.77	0.67
3:D:115:SER:HB2	3:D:138:ASN:HB3	1.75	0.66
2:E:216:HIS:HE1	2:E:218:PRO:HG2	1.59	0.66
1:A:253:LEU:HD11	1:A:283:VAL:HG12	1.76	0.66
2:E:135:PRO:HD3	2:E:216:HIS:CD2	2.31	0.66
1:A:58:PRO:HG2	1:A:423:ARG:NH1	2.11	0.66
1:A:281:LYS:HD2	1:A:281:LYS:O	1.96	0.66
3:D:33:VAL:HG12	3:D:51:THR:HG23	1.78	0.65
2:E:22:CYS:HB3	2:E:79:ALA:HB3	1.78	0.65
2:E:154:LEU:HD21	2:E:210:TYR:HD2	1.60	0.65
1:B:387:VAL:HG21	1:B:480:ILE:HD13	1.78	0.65
2:C:14:PRO:HD2	2:C:129:SER:HB3	1.79	0.65
2:C:172:SER:H	2:C:213:ASN:HD21	1.44	0.65
2:E:55:TYR:HE2	2:E:105:TRP:HA	1.61	0.64
1:A:387:VAL:HG21	1:A:480:ILE:HD13	1.78	0.64
3:D:165:THR:HG22	3:D:175:SER:H	1.63	0.64
1:B:170:LEU:HD22	1:B:277:GLU:HG3	1.80	0.64
1:B:118:THR:CG2	1:B:171:SER:O	2.46	0.63
3:D:143:ARG:NH1	3:D:164:VAL:HG21	2.13	0.63
1:A:573:ASN:HD22	1:A:632:LYS:HB3	1.63	0.63
2:C:67:ARG:O	2:C:68:PHE:CD1	2.50	0.63
3:F:29:VAL:HG12	3:F:29:VAL:O	1.98	0.63
1:A:423:ARG:HH11	1:A:423:ARG:HG3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.81	0.63
1:B:528:ASN:C	1:B:528:ASN:HD22	2.04	0.63
1:B:114:LEU:O	1:B:114:LEU:CG	2.47	0.63
2:C:6:GLU:OE2	2:C:120:GLY:HA3	1.98	0.63
3:D:116:VAL:HG22	3:D:137:LEU:HD22	1.82	0.62
1:B:864:GLU:HG3	1:B:986:LEU:HD21	1.81	0.62
2:C:55:TYR:CE2	2:C:105:TRP:HA	2.35	0.62
2:E:83:MET:HE1	2:E:125:VAL:HG21	1.81	0.61
2:C:12:VAL:HG11	2:C:18:LEU:HG	1.82	0.61
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.81	0.61
1:B:423:ARG:HH11	1:B:423:ARG:CG	2.13	0.61
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.82	0.61
1:A:99:ASP:O	1:A:217:LYS:NZ	2.32	0.61
2:E:209:THR:O	2:E:209:THR:HG23	2.00	0.60
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.83	0.60
1:B:47:ILE:HD11	1:B:272:VAL:HG22	1.83	0.60
1:A:388:GLU:OE2	1:A:509:VAL:HG22	2.02	0.60
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.84	0.60
2:C:55:TYR:HE2	2:C:105:TRP:HA	1.66	0.60
3:F:142:PRO:HD2	3:F:199:HIS:NE2	2.17	0.59
1:A:910:GLU:OE1	1:A:920:ARG:NH1	2.35	0.59
1:B:119:LYS:O	1:B:119:LYS:HG2	2.02	0.59
1:B:832:ILE:HB	1:B:851:GLN:HB3	1.84	0.59
1:B:635:ASN:HA	1:B:638:GLN:HB2	1.84	0.59
2:E:180:HIS:HB2	2:E:197:VAL:HG12	1.83	0.59
1:B:657:LYS:HE3	1:B:661:ILE:HD11	1.84	0.59
1:A:202:PHE:CZ	1:A:206:LYS:HE3	2.38	0.59
1:B:115:PHE:CD1	1:B:168:PHE:HE2	2.17	0.59
3:D:6:GLN:HB3	3:D:101:GLN:HE22	1.68	0.59
1:B:635:ASN:ND2	1:B:732:ASN:O	2.36	0.59
1:A:304:ILE:HB	1:A:481:VAL:HG22	1.84	0.58
2:E:216:HIS:CE1	2:E:218:PRO:CD	2.86	0.58
2:C:170:TRP:CZ3	2:C:212:CYS:HB3	2.38	0.58
1:B:251:SER:OG	1:B:280:ASN:HB2	2.03	0.58
2:C:67:ARG:C	2:C:68:PHE:CD1	2.81	0.58
2:C:135:PRO:HD2	2:C:221:THR:HG21	1.86	0.58
3:F:143:ARG:HB3	3:F:143:ARG:NH1	2.17	0.58
1:B:76:LEU:HB3	1:B:257:VAL:HG23	1.86	0.58
2:C:142:PRO:HD2	2:C:229:PRO:HA	1.85	0.58
3:F:146:LYS:HB3	3:F:198:THR:HG23	1.85	0.58
1:A:357:ASN:HB2	1:A:378:ASP:OD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ARG:NH1	1:A:963:MET:O	2.36	0.57
2:E:38:ARG:NE	2:E:46:GLU:OE1	2.33	0.57
3:F:140:PHE:HE1	3:F:143:ARG:HA	1.69	0.57
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.86	0.57
2:E:91:THR:HG1	2:E:127:VAL:H	1.52	0.57
3:F:79:GLN:HB3	3:F:80:PRO:HD2	1.86	0.57
1:B:573:ASN:HD22	1:B:632:LYS:HB3	1.67	0.57
3:F:18:ARG:NH2	3:F:74:THR:HG21	2.19	0.57
3:F:38:GLN:O	3:F:84:ALA:HB1	2.05	0.56
1:B:528:ASN:HD22	1:B:530:PHE:H	1.53	0.56
1:B:799:MET:HE3	1:B:1008:VAL:HG22	1.87	0.56
3:F:6:GLN:NE2	3:F:88:CYS:SG	2.78	0.56
1:B:99:ASP:OD1	1:B:99:ASP:N	2.38	0.56
1:B:326:TYR:CE2	1:B:443:TYR:HB3	2.40	0.56
2:E:55:TYR:CE2	2:E:105:TRP:HA	2.39	0.56
1:B:765:ARG:HG3	1:B:765:ARG:HH11	1.69	0.56
1:B:771:LEU:H	1:B:796:GLN:HE22	1.54	0.56
3:F:35:TRP:CH2	3:F:88:CYS:HB3	2.41	0.55
1:A:541:GLU:OE2	1:A:542:LYS:HE3	2.06	0.55
3:D:165:THR:CG2	3:D:175:SER:H	2.19	0.55
1:A:312:ASN:HD22	1:A:378:ASP:HA	1.71	0.55
1:A:321:ASP:O	1:A:324:LYS:NZ	2.39	0.55
1:B:153:VAL:HG22	1:B:154:SER:H	1.72	0.55
1:B:251:SER:HB3	1:B:278:VAL:HG12	1.87	0.55
3:D:38:GLN:O	3:D:84:ALA:HB1	2.07	0.55
1:A:75:VAL:HG11	1:A:271:VAL:HG11	1.89	0.55
1:B:348:SER:HB2	1:B:606:GLU:OE2	2.06	0.55
1:B:365:GLU:HG2	1:B:371:MET:HG2	1.89	0.55
2:E:2:VAL:HG22	2:E:27:PHE:HD1	1.72	0.55
2:C:83:MET:HB3	2:C:86:LEU:HD21	1.89	0.55
3:D:194:ALA:HA	3:D:209:SER:HA	1.88	0.55
1:B:888:ALA:O	1:B:891:ILE:HG13	2.07	0.54
3:D:143:ARG:O	3:D:143:ARG:NE	2.38	0.54
2:E:11:LEU:HD12	2:E:163:PRO:HD3	1.89	0.54
1:B:538:LEU:HD22	1:B:734:THR:HG23	1.90	0.54
1:B:88:ALA:HB3	1:B:151:PHE:CZ	2.42	0.54
1:B:765:ARG:HH11	1:B:765:ARG:CG	2.21	0.54
1:A:517:ASP:OD1	1:A:517:ASP:N	2.25	0.54
2:E:135:PRO:HD2	2:E:221:THR:OG1	2.05	0.54
2:E:138:PHE:CG	3:F:125:GLN:HG3	2.42	0.54
1:B:47:ILE:HG22	1:B:48:LYS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:216:HIS:CE1	2:E:218:PRO:HG2	2.40	0.54
3:F:109:ARG:HH11	3:F:109:ARG:HB2	1.71	0.54
3:F:40:PRO:HG2	3:F:166:GLU:HG2	1.89	0.54
1:B:643:LYS:HE3	1:B:647:GLU:CD	2.33	0.54
2:E:59:SER:HB2	3:F:95:PHE:HB3	1.89	0.54
1:A:635:ASN:ND2	1:A:732:ASN:O	2.41	0.54
3:D:6:GLN:HB3	3:D:101:GLN:NE2	2.23	0.54
2:C:197:VAL:HG11	3:D:136:LEU:HD13	1.89	0.53
2:E:104:TYR:CD1	2:E:104:TYR:C	2.85	0.53
2:E:4:LEU:HD21	2:E:27:PHE:HZ	1.72	0.53
2:C:4:LEU:HD21	2:C:27:PHE:CZ	2.44	0.53
2:C:32:TYR:CZ	2:C:102:MET:HG2	2.43	0.53
1:A:561:PHE:HE1	1:A:733:ILE:HD12	1.74	0.53
2:C:4:LEU:HD21	2:C:27:PHE:HZ	1.74	0.53
1:B:436:LYS:HE3	1:B:453:GLU:OE2	2.09	0.53
1:B:322:LEU:HA	1:B:325:TYR:CD2	2.44	0.52
2:C:11:LEU:HD11	2:C:162:PHE:HE1	1.74	0.52
1:A:896:LYS:HD2	1:A:897:PRO:HD2	1.91	0.52
1:A:519:ASN:OD1	1:A:521:LYS:HG2	2.09	0.52
1:B:434:THR:O	1:B:437:ILE:O	2.28	0.52
1:B:173:LEU:O	1:B:174:PHE:HD1	1.92	0.52
1:B:938:LYS:O	1:B:942:GLU:HG2	2.10	0.52
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.91	0.52
1:B:59:GLU:CD	1:B:59:GLU:O	2.53	0.52
2:E:186:LEU:HG	2:E:192:TYR:CE1	2.45	0.52
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.45	0.51
1:A:706:ASP:OD1	1:B:756:LYS:NZ	2.38	0.51
1:A:963:MET:SD	1:A:964:ASP:N	2.84	0.51
2:C:64:VAL:HG12	2:C:67:ARG:NH2	2.25	0.51
1:B:561:PHE:HE1	1:B:733:ILE:HD12	1.76	0.51
2:C:157:LEU:HD13	2:C:195:SER:HB3	1.92	0.51
1:A:316:THR:HB	1:A:374:ILE:HG22	1.92	0.51
1:B:346:LEU:HD21	1:B:394:MET:HG2	1.91	0.51
2:E:211:ILE:HG22	2:E:226:LYS:HA	1.92	0.51
2:C:83:MET:HE1	2:C:125:VAL:HG11	1.92	0.51
1:A:557:SER:OG	1:A:746:GLU:OE2	2.20	0.51
1:B:423:ARG:CG	1:B:423:ARG:NH1	2.73	0.51
1:B:607:TYR:CZ	1:B:644:LYS:HD2	2.46	0.51
3:D:212:ARG:HB3	3:D:212:ARG:CZ	2.40	0.51
2:E:100:ARG:HB3	2:E:117:ASP:HB3	1.92	0.51
2:C:59:SER:HB2	3:D:95:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:161:GLN:HG3	3:F:179:THR:HB	1.91	0.51
1:A:465:GLU:HG2	2:C:105:TRP:CZ3	2.43	0.50
3:D:51:THR:HG21	3:D:71:PHE:HD2	1.76	0.50
1:B:528:ASN:ND2	1:B:528:ASN:C	2.69	0.50
1:A:162:LEU:HD23	1:A:270:LEU:HG	1.92	0.50
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.92	0.50
3:D:11:LEU:HD13	3:D:19:VAL:HG13	1.92	0.50
3:F:29:VAL:C	3:F:31:SER:H	2.19	0.50
3:D:35:TRP:CH2	3:D:88:CYS:HB3	2.47	0.50
1:A:52:ASN:O	1:A:54:ILE:HG12	2.11	0.50
1:A:643:LYS:HE2	1:A:744:MET:SD	2.52	0.50
1:B:311:ARG:HD3	1:B:384:LEU:HB2	1.94	0.50
2:E:154:LEU:HD21	2:E:210:TYR:CD2	2.45	0.50
1:B:311:ARG:NH2	1:B:381:GLU:OE1	2.45	0.50
1:A:446:LEU:O	1:A:449:VAL:HG22	2.12	0.49
2:C:158:VAL:HB	2:C:194:LEU:HD23	1.94	0.49
2:E:121:GLN:H	2:E:121:GLN:CD	2.19	0.49
1:A:123:LYS:HB2	1:A:126:GLU:HB2	1.95	0.49
1:B:896:LYS:O	1:B:898:LYS:NZ	2.41	0.49
1:B:143:SER:OG	1:B:146:HIS:HB2	2.12	0.49
2:C:162:PHE:HB2	2:C:191:LEU:HD22	1.93	0.49
2:E:113:PRO:HG2	3:F:32:ALA:O	2.12	0.49
2:C:132:THR:HG23	2:C:162:PHE:O	2.12	0.49
1:B:395:PHE:CD2	1:B:513:TRP:HB3	2.48	0.49
3:D:116:VAL:HG21	3:D:197:VAL:HG21	1.93	0.49
3:F:35:TRP:CD2	3:F:73:LEU:HB2	2.47	0.49
3:D:115:SER:O	3:D:138:ASN:HB2	2.12	0.49
1:B:86:SER:HB3	1:B:158:LEU:HG	1.94	0.49
3:D:150:LYS:HB2	3:D:194:ALA:HB3	1.95	0.49
2:E:54:TYR:HD2	2:E:103:TYR:CD1	2.30	0.49
1:B:48:LYS:HG2	1:B:49:ARG:N	2.25	0.48
1:B:90:LEU:HD12	1:B:256:VAL:HG22	1.94	0.48
3:F:122:SER:OG	3:F:125:GLN:HB2	2.13	0.48
1:B:601:LYS:HD3	1:B:620:LEU:O	2.13	0.48
2:E:45:LEU:HD12	3:F:87:TYR:CD2	2.48	0.48
1:A:177:SER:OG	1:A:181:ARG:NH1	2.45	0.48
1:A:344:GLY:HA3	1:A:523:LYS:HG2	1.94	0.48
1:B:588:LEU:HD22	1:B:711:ARG:HH11	1.78	0.48
1:B:173:LEU:O	1:B:174:PHE:HB2	2.12	0.48
1:A:81:PRO:HA	1:A:261:ARG:HD3	1.95	0.48
3:D:7:SER:HA	3:D:8:PRO:HA	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ARG:HH11	1:A:423:ARG:HG2	1.77	0.48
1:B:519:ASN:ND2	1:B:519:ASN:C	2.64	0.48
2:E:170:TRP:CZ3	2:E:212:CYS:HB3	2.49	0.48
2:C:32:TYR:CZ	2:C:98:ARG:NH2	2.82	0.48
3:D:10:SER:HB2	3:D:104:LYS:O	2.14	0.48
3:D:115:SER:CB	3:D:138:ASN:HB2	2.36	0.48
1:B:893:ARG:HA	1:B:893:ARG:HH11	1.79	0.47
3:F:108:LYS:HA	3:F:141:TYR:OH	2.14	0.47
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.39	0.47
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.96	0.47
2:E:216:HIS:CE1	2:E:218:PRO:CG	2.97	0.47
1:B:927:TYR:O	1:B:930:THR:HB	2.13	0.47
3:D:147:VAL:HA	3:D:196:GLU:O	2.14	0.47
2:E:73:ASP:OD2	2:E:76:LYS:HG3	2.14	0.47
1:B:319:ILE:HD11	1:B:371:MET:HE2	1.97	0.47
1:B:437:ILE:O	1:B:438:ALA:HB3	2.15	0.47
2:C:54:TYR:HD2	2:C:103:TYR:HD1	1.63	0.47
2:E:135:PRO:HA	2:E:160:ASP:O	2.14	0.47
3:F:22:THR:HG22	3:F:72:THR:OG1	2.14	0.47
2:E:22:CYS:HB2	2:E:36:TRP:CZ2	2.49	0.47
1:B:315:VAL:HG21	1:B:394:MET:HE1	1.97	0.47
1:B:671:ASN:HA	1:B:701:LYS:HZ1	1.80	0.47
3:D:80:PRO:HA	3:D:83:PHE:HE2	1.80	0.47
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.97	0.46
1:B:438:ALA:HA	1:B:441:LEU:HG	1.96	0.46
1:B:777:PHE:HD1	1:B:990:GLU:HB3	1.79	0.46
1:A:879:GLU:OE2	1:A:883:GLN:HG2	2.15	0.46
2:E:139:PRO:HB2	2:E:227:VAL:HG22	1.97	0.46
2:E:200:VAL:HG11	2:E:210:TYR:CE2	2.49	0.46
1:B:93:HIS:O	1:B:94:ILE:HG12	2.16	0.46
1:B:336:HIS:CD2	1:B:414:LEU:HD11	2.50	0.46
1:B:444:TYR:CD2	1:B:452:ALA:HB1	2.51	0.46
1:B:638:GLN:N	1:B:639:PRO:HD2	2.30	0.46
2:C:137:VAL:HG22	2:C:214:VAL:HG21	1.98	0.46
3:F:118:ILE:HG13	3:F:119:PHE:N	2.31	0.46
1:A:680:GLN:HA	1:A:683:MET:HE3	1.98	0.46
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.98	0.46
2:E:12:VAL:HG11	2:E:18:LEU:HG	1.98	0.46
3:F:29:VAL:C	3:F:31:SER:N	2.72	0.46
1:B:684:TYR:CZ	1:B:688:LEU:HD11	2.51	0.46
3:D:36:TYR:CE2	3:D:46:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:199:HIS:HB3	3:D:202:LEU:HD22	1.97	0.46
2:E:4:LEU:HD13	2:E:22:CYS:SG	2.55	0.46
1:B:54:ILE:HG22	1:B:450:LEU:HD22	1.98	0.46
1:B:93:HIS:C	1:B:94:ILE:HG12	2.40	0.46
2:C:38:ARG:NE	2:C:46:GLU:OE1	2.41	0.46
1:A:460:ARG:NH2	2:C:101:VAL:HB	2.30	0.46
1:A:541:GLU:HG2	1:A:563:GLN:OE1	2.16	0.46
1:B:173:LEU:C	1:B:173:LEU:CD2	2.85	0.46
1:A:85:LYS:HG3	1:A:430:PRO:HG2	1.97	0.45
1:A:718:GLN:O	1:A:721:SER:OG	2.32	0.45
2:C:54:TYR:CD1	2:C:54:TYR:C	2.94	0.45
3:F:149:TRP:HA	3:F:194:ALA:O	2.16	0.45
1:A:170:LEU:HD21	1:A:277:GLU:HG2	1.97	0.45
1:A:251:SER:HB3	1:A:278:VAL:HG12	1.98	0.45
1:A:299:LYS:HD2	1:A:510:ILE:HD13	1.98	0.45
1:A:346:LEU:HD21	1:A:394:MET:HG2	1.97	0.45
1:B:115:PHE:CD1	1:B:168:PHE:CD2	3.04	0.45
1:B:709:LEU:HB3	1:B:710:PRO:CD	2.47	0.45
2:E:28:ASN:C	2:E:30:SER:H	2.24	0.45
1:A:253:LEU:HD11	1:A:283:VAL:CG1	2.44	0.45
2:C:178:GLY:O	2:C:198:VAL:HA	2.16	0.45
3:F:65:SER:OG	3:F:72:THR:HB	2.16	0.45
1:B:391:ILE:HA	1:B:394:MET:HE2	1.98	0.45
1:B:689:LEU:C	1:B:690:MET:HE2	2.41	0.45
2:C:4:LEU:HD13	2:C:22:CYS:SG	2.57	0.45
3:F:176:LEU:HD12	3:F:177:SER:H	1.81	0.45
1:A:319:ILE:HB	1:A:320:PRO:HD2	1.98	0.45
1:B:436:LYS:HE3	1:B:453:GLU:CD	2.42	0.45
1:B:856:PRO:HG2	1:B:959:LEU:HD23	1.98	0.45
2:E:47:TRP:CD2	3:F:97:ILE:HB	2.51	0.45
1:A:771:LEU:HB2	1:A:796:GLN:NE2	2.31	0.45
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.52	0.45
1:A:116:LEU:HD13	1:A:178:ALA:HB1	1.99	0.45
1:B:325:TYR:HE1	2:E:103:TYR:CB	2.30	0.45
1:B:648:LYS:HA	1:B:648:LYS:HD3	1.72	0.45
2:E:214:VAL:HB	2:E:223:VAL:HG13	1.99	0.45
2:E:23:ALA:CA	2:E:78:THR:HG23	2.44	0.45
1:A:769:VAL:HA	1:A:1004:LEU:HD23	1.98	0.45
1:A:927:TYR:O	1:A:930:THR:HB	2.16	0.45
1:B:896:LYS:HB2	1:B:896:LYS:HE2	1.50	0.45
1:A:466:MET:HB2	2:C:105:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:155:GLY:HA2	2:E:170:TRP:CH2	2.52	0.44
2:E:200:VAL:HG21	2:E:210:TYR:HE2	1.83	0.44
1:B:93:HIS:CE1	1:B:442:HIS:HB3	2.52	0.44
2:C:54:TYR:HD1	2:C:54:TYR:O	2.00	0.44
3:D:59:PRO:HG2	3:D:62:PHE:CE2	2.52	0.44
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.98	0.44
1:A:917:ASN:CG	1:A:920:ARG:HB2	2.42	0.44
2:C:140:LEU:HB3	3:D:119:PHE:CD1	2.52	0.44
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.16	0.44
1:B:854:LYS:HE3	1:B:858:TYR:CE2	2.52	0.44
3:D:35:TRP:CZ3	3:D:88:CYS:HB3	2.53	0.44
2:C:159:LYS:NZ	2:C:159:LYS:HB3	2.32	0.44
2:E:217:LYS:N	2:E:218:PRO:CD	2.81	0.44
3:F:35:TRP:CZ3	3:F:88:CYS:HB3	2.53	0.44
3:F:119:PHE:HA	3:F:120:PRO:HD3	1.82	0.44
3:D:35:TRP:HB2	3:D:48:ILE:HB	1.98	0.44
3:F:14:SER:O	3:F:17:ASP:HB2	2.18	0.44
3:F:36:TYR:CE2	3:F:46:LEU:HD13	2.52	0.44
1:A:206:LYS:O	1:A:216:SER:HA	2.17	0.44
1:B:411:PHE:CE2	1:B:459:PHE:HB2	2.53	0.44
2:E:6:GLU:N	2:E:6:GLU:OE1	2.51	0.44
2:E:31:SER:O	2:E:102:MET:O	2.36	0.44
3:F:50:SER:C	3:F:52:SER:H	2.25	0.44
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.68	0.44
1:B:448:GLU:O	1:B:452:ALA:N	2.50	0.44
1:B:777:PHE:CD2	1:B:998:PHE:HE1	2.34	0.44
1:A:62:ARG:HG2	1:A:80:ASP:HB2	2.00	0.43
1:B:140:ALA:HB2	1:B:149:TYR:HA	2.00	0.43
1:B:872:LYS:HD2	1:B:876:ASP:OD2	2.18	0.43
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.53	0.43
1:A:771:LEU:H	1:A:796:GLN:NE2	2.09	0.43
1:B:559:LEU:HD22	1:B:742:MET:HB2	2.00	0.43
3:D:59:PRO:HG2	3:D:62:PHE:HE2	1.84	0.43
2:E:116:MET:HE2	3:F:89:GLN:OE1	2.18	0.43
2:E:182:PHE:CZ	3:F:177:SER:HB2	2.53	0.43
1:A:472:ARG:C	1:A:474:GLU:H	2.27	0.43
1:B:131:LEU:O	1:B:136:GLY:N	2.43	0.43
2:C:167:THR:OG1	2:C:215:ASN:HB3	2.19	0.43
1:B:630:SER:OG	1:B:632:LYS:HE3	2.19	0.43
1:B:649:MET:HE3	1:B:649:MET:HB2	1.91	0.43
2:E:47:TRP:CE2	3:F:97:ILE:HB	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:GLU:O	1:A:933:LYS:NZ	2.43	0.43
1:B:446:LEU:O	1:B:449:VAL:HG12	2.19	0.43
2:E:54:TYR:CD1	2:E:54:TYR:C	2.96	0.43
3:F:113:ALA:HA	3:F:114:PRO:HD3	1.82	0.43
3:F:168:ASP:OD1	3:F:169:SER:N	2.52	0.43
1:A:90:LEU:HD13	1:A:169:PHE:CE2	2.54	0.43
1:A:181:ARG:O	1:A:184:ASN:HB3	2.18	0.43
1:B:308:LYS:HG2	1:B:675:ALA:HB3	2.01	0.43
1:B:466:MET:HB2	2:E:105:TRP:CD2	2.52	0.43
1:B:806:MET:O	1:B:810:LEU:HB2	2.19	0.43
2:E:31:SER:HB2	2:E:103:TYR:CE1	2.54	0.43
2:E:54:TYR:HD1	2:E:54:TYR:O	2.01	0.43
1:A:649:MET:HE3	1:A:649:MET:HB2	1.95	0.43
1:B:86:SER:OG	1:B:155:HIS:HA	2.18	0.43
1:B:115:PHE:CE1	1:B:168:PHE:CE2	3.07	0.43
2:C:141:ALA:HA	2:C:142:PRO:HD3	1.82	0.43
2:C:164:GLU:HA	2:C:165:PRO:HA	1.73	0.43
2:C:215:ASN:OD1	2:C:222:LYS:HG2	2.19	0.43
1:A:313:LEU:HD22	1:A:387:VAL:HG13	2.01	0.43
1:B:130:PHE:HE1	1:B:161:ALA:HB2	1.83	0.43
1:B:252:ASN:HB3	1:B:280:ASN:ND2	2.34	0.43
3:F:7:SER:HA	3:F:8:PRO:HA	1.56	0.43
1:A:48:LYS:HB2	1:A:48:LYS:HE3	1.75	0.42
1:B:173:LEU:O	1:B:174:PHE:CD1	2.70	0.42
3:D:155:LEU:HB3	3:D:157:SER:HB2	2.00	0.42
3:F:35:TRP:HA	3:F:87:TYR:O	2.19	0.42
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.48	0.42
1:B:92:VAL:O	1:B:92:VAL:CG1	2.59	0.42
3:D:59:PRO:HB3	3:D:61:ARG:NH1	2.34	0.42
3:F:50:SER:C	3:F:52:SER:N	2.77	0.42
1:A:690:MET:O	1:A:768:GLU:HG3	2.19	0.42
1:B:307:ILE:HD11	1:B:785:VAL:HG13	2.00	0.42
2:E:55:TYR:CE2	2:E:105:TRP:HD1	2.37	0.42
3:F:19:VAL:HG21	3:F:78:LEU:HD22	2.01	0.42
3:F:193:TYR:HB2	3:F:210:PHE:CZ	2.53	0.42
1:A:903:GLU:OE1	1:A:907:TYR:OH	2.29	0.42
1:B:130:PHE:CE1	1:B:161:ALA:HB2	2.55	0.42
2:E:33:SER:HB2	2:E:99:ASP:OD2	2.19	0.42
2:E:164:GLU:HG3	2:E:192:TYR:CE2	2.55	0.42
1:A:946:VAL:HA	1:A:951:ARG:CZ	2.50	0.42
1:A:46:ALA:O	1:A:70:ALA:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:212:ARG:HB3	3:D:212:ARG:NH1	2.35	0.42
2:E:98:ARG:HD2	2:E:99:ASP:O	2.19	0.42
1:A:102:ASN:O	1:A:102:ASN:ND2	2.45	0.42
1:A:247:ALA:O	1:A:283:VAL:HG21	2.20	0.42
1:B:642:LEU:O	1:B:646:ILE:HG12	2.19	0.42
1:B:528:ASN:O	1:B:531:ILE:HG12	2.19	0.42
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.55	0.42
3:D:47:LEU:HD11	3:D:86:TYR:HE1	1.85	0.42
3:D:141:TYR:CD1	3:D:142:PRO:HA	2.55	0.42
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.83	0.42
2:C:2:VAL:HG22	2:C:27:PHE:HD1	1.84	0.42
2:E:139:PRO:CB	2:E:227:VAL:HG22	2.49	0.42
3:D:162:GLU:HG2	3:D:178:SER:HA	2.02	0.42
2:E:162:PHE:HB2	2:E:191:LEU:HD22	2.02	0.42
3:F:21:ILE:O	3:F:72:THR:HG23	2.19	0.42
1:A:56:LYS:NZ	1:A:62:ARG:O	2.47	0.41
1:A:80:ASP:O	1:A:83:THR:HG22	2.20	0.41
1:B:580:SER:HA	1:B:581:PRO:HD2	1.85	0.41
3:D:50:SER:OG	3:D:53:SER:OG	2.24	0.41
2:E:36:TRP:HD1	2:E:70:ILE:HD11	1.85	0.41
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.91	0.41
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.87	0.41
2:C:100:ARG:HG3	2:C:117:ASP:HB3	2.02	0.41
2:E:12:VAL:HG23	2:E:127:VAL:HG22	2.01	0.41
2:E:166:VAL:HG12	2:E:216:HIS:HA	2.02	0.41
1:A:871:GLU:HB2	1:A:940:TYR:CE2	2.56	0.41
2:C:33:SER:HB2	2:C:99:ASP:OD2	2.20	0.41
2:E:67:ARG:HB3	2:E:68:PHE:CD1	2.48	0.41
2:E:97:ALA:HB2	2:E:119:TRP:CG	2.56	0.41
2:E:164:GLU:HA	2:E:165:PRO:HA	1.90	0.41
3:D:69:THR:HB	3:D:70:ASP:H	1.57	0.41
1:A:63:GLU:HB3	1:A:264:LEU:HD11	2.02	0.41
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.56	0.41
1:A:468:LEU:HD12	1:A:468:LEU:HA	1.89	0.41
1:A:765:ARG:HH11	1:A:765:ARG:CG	2.20	0.41
1:B:80:ASP:O	1:B:83:THR:HG22	2.21	0.41
2:C:54:TYR:C	2:C:54:TYR:HD1	2.27	0.41
3:F:85:THR:HG23	3:F:104:LYS:HD2	2.01	0.41
1:B:437:ILE:O	1:B:438:ALA:CB	2.69	0.41
1:B:940:TYR:CE2	1:B:945:ALA:HB2	2.55	0.41
3:F:24:ARG:HD2	3:F:70:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:112:ALA:HB3	3:F:140:PHE:HA	2.03	0.41
3:F:159:ASN:ND2	3:F:181:THR:OG1	2.53	0.41
3:F:194:ALA:CB	3:F:209:SER:HB3	2.50	0.41
1:A:172:PRO:HG2	1:A:174:PHE:CE2	2.55	0.41
1:A:925:VAL:O	1:A:929:LYS:HG3	2.21	0.41
1:B:89:ALA:HA	1:B:149:TYR:O	2.20	0.41
1:B:153:VAL:HG22	1:B:154:SER:N	2.35	0.41
1:B:397:TYR:O	1:B:400:LYS:HB3	2.21	0.41
1:B:540:LEU:HA	1:B:540:LEU:HD12	1.86	0.41
3:D:35:TRP:CE2	3:D:73:LEU:HB2	2.55	0.41
3:D:138:ASN:HB3	3:D:139:ASN:H	1.73	0.41
1:A:933:LYS:O	1:A:937:ILE:HG13	2.21	0.41
1:B:357:ASN:HB2	1:B:378:ASP:OD2	2.21	0.41
1:B:765:ARG:CG	1:B:765:ARG:NH1	2.80	0.41
1:B:791:ILE:HG22	1:B:850:ILE:HB	2.02	0.41
1:B:906:LYS:HB3	1:B:906:LYS:HE3	1.83	0.41
2:C:3:GLN:HG3	2:C:25:SER:OG	2.20	0.41
3:D:29:VAL:HB	3:D:30:SER:H	1.72	0.41
3:F:83:PHE:O	3:F:83:PHE:CG	2.73	0.41
1:A:474:GLU:H	1:A:474:GLU:HG2	1.62	0.41
1:A:616:LEU:HA	1:A:616:LEU:HD12	1.77	0.41
2:C:51:ILE:HB	2:C:70:ILE:HD13	2.02	0.41
2:C:170:TRP:CE3	2:C:212:CYS:HB3	2.55	0.41
2:C:23:ALA:CA	2:C:78:THR:HG23	2.47	0.40
2:E:138:PHE:HB3	3:F:122:SER:OG	2.21	0.40
2:E:178:GLY:O	2:E:198:VAL:HA	2.20	0.40
1:A:103:ILE:HD11	1:A:240:GLU:HG3	2.03	0.40
1:A:934:GLU:H	1:A:934:GLU:HG2	1.38	0.40
1:B:163:ASP:HA	1:B:274:LEU:HD13	2.03	0.40
1:B:319:ILE:HB	1:B:320:PRO:HD2	2.02	0.40
2:E:181:THR:HG22	2:E:196:SER:OG	2.21	0.40
1:A:832:ILE:HB	1:A:851:GLN:HB3	2.03	0.40
1:B:819:ALA:O	1:B:823:LEU:HB2	2.22	0.40
1:B:868:ILE:HG13	1:B:869:THR:N	2.37	0.40
1:B:872:LYS:HG3	1:B:873:SER:N	2.36	0.40
3:D:142:PRO:HB2	3:D:144:GLU:HG2	2.03	0.40
3:F:109:ARG:HG2	3:F:141:TYR:CD1	2.56	0.40
1:A:1007:LEU:HD23	1:B:1000:ARG:HG2	2.03	0.40
1:B:709:LEU:HD12	1:B:709:LEU:HA	1.88	0.40
2:C:211:ILE:HD13	2:C:226:LYS:HB3	2.03	0.40
2:C:135:PRO:HA	2:C:160:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:PHE:CD1	3:D:107:ILE:HG22	2.57	0.40
3:D:113:ALA:HA	3:D:114:PRO:HD3	1.84	0.40
3:F:39:LYS:NZ	3:F:81:GLU:O	2.43	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	922/990 (93%)	886 (96%)	35 (4%)	1 (0%)	48	76
1	B	845/990 (85%)	804 (95%)	38 (4%)	3 (0%)	30	58
2	C	206/263 (78%)	188 (91%)	15 (7%)	3 (2%)	8	29
2	E	199/263 (76%)	178 (89%)	19 (10%)	2 (1%)	12	38
3	D	187/239 (78%)	165 (88%)	21 (11%)	1 (0%)	24	52
3	F	191/239 (80%)	162 (85%)	28 (15%)	1 (0%)	24	52
All	All	2550/2984 (86%)	2383 (94%)	156 (6%)	11 (0%)	30	58

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	138	ASN
1	A	282	ASN
1	B	95	GLY
1	B	172	PRO
1	B	1010	PRO
2	C	122	GLY
3	F	40	PRO
2	C	165	PRO
2	E	165	PRO

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Mol	Chain	Res	Type
2	E	171	ASN
2	C	85	SER

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	832/879 (95%)	771 (93%)	61 (7%)	13	39
1	B	768/879 (87%)	710 (92%)	58 (8%)	12	38
2	C	181/220 (82%)	161 (89%)	20 (11%)	6	22
2	E	176/220 (80%)	156 (89%)	20 (11%)	5	20
3	D	178/210 (85%)	154 (86%)	24 (14%)	4	15
3	F	176/210 (84%)	154 (88%)	22 (12%)	4	17
All	All	2311/2618 (88%)	2106 (91%)	205 (9%)	9	31

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	97	LEU
1	A	111	GLU
1	A	192	LYS
1	A	201	LEU
1	A	223	LYS
1	A	226	LEU
1	A	273	LYS
1	A	283	VAL
1	A	316	THR
1	A	324	LYS
1	A	347	LEU
1	A	353	LYS
1	A	356	VAL
1	A	412	GLN
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	423	ARG
1	A	440	ILE
1	A	446	LEU
1	A	450	LEU
1	A	468	LEU
1	A	474	GLU
1	A	486	GLU
1	A	499	GLN
1	A	508	GLU
1	A	517	ASP
1	A	524	LEU
1	A	531	ILE
1	A	542	LYS
1	A	543	GLU
1	A	595	LEU
1	A	597	LEU
1	A	600	LEU
1	A	603	SER
1	A	616	LEU
1	A	632	LYS
1	A	642	LEU
1	A	648	LYS
1	A	660	GLU
1	A	712	LEU
1	A	728	LEU
1	A	733	ILE
1	A	765	ARG
1	A	771	LEU
1	A	781	GLN
1	A	799	MET
1	A	810	LEU
1	A	823	LEU
1	A	846	LEU
1	A	859	LEU
1	A	867	LEU
1	A	871	GLU
1	A	889	LEU
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	934	GLU
1	A	954	VAL

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Mol	Chain	Res	Type
1	A	979	ASN
1	A	993	GLN
1	A	1007	LEU
1	B	111	GLU
1	B	158	LEU
1	B	173	LEU
1	B	270	LEU
1	B	273	LYS
1	B	316	THR
1	B	347	LEU
1	B	348	SER
1	B	353	LYS
1	B	356	VAL
1	B	412	GLN
1	B	414	LEU
1	B	423	ARG
1	B	435	SER
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	466	MET
1	B	468	LEU
1	B	486	GLU
1	B	499	GLN
1	B	508	GLU
1	B	517	ASP
1	B	519	ASN
1	B	524	LEU
1	B	542	LYS
1	B	595	LEU
1	B	597	LEU
1	B	600	LEU
1	B	603	SER
1	B	616	LEU
1	B	629	LEU
1	B	632	LYS
1	B	642	LEU
1	B	648	LYS
1	B	728	LEU
1	B	733	ILE
1	B	765	ARG
1	B	771	LEU

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Mol	Chain	Res	Type
1	B	781	GLN
1	B	799	MET
1	B	810	LEU
1	B	853	GLU
1	B	859	LEU
1	B	861	SER
1	B	867	LEU
1	B	871	GLU
1	B	872	LYS
1	B	879	GLU
1	B	889	LEU
1	B	928	LEU
1	B	930	THR
1	B	931	LEU
1	B	934	GLU
1	B	938	LYS
1	B	964	ASP
1	B	993	GLN
1	B	1011	HIS
2	C	2	VAL
2	C	7	SER
2	C	54	TYR
2	C	81	LEU
2	C	94	TYR
2	C	109	LYS
2	C	110	TYR
2	C	123	THR
2	C	125	VAL
2	C	126	THR
2	C	159	LYS
2	C	175	LEU
2	C	185	VAL
2	C	187	GLN
2	C	195	SER
2	C	211	ILE
2	C	213	ASN
2	C	217	LYS
2	C	223	VAL
2	C	230	LYS
3	D	17	ASP
3	D	33	VAL
3	D	65	SER

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Mol	Chain	Res	Type
3	D	72	THR
3	D	95	PHE
3	D	97	ILE
3	D	98	THR
3	D	107	ILE
3	D	108	LYS
3	D	109	ARG
3	D	110	THR
3	D	122	SER
3	D	132	SER
3	D	143	ARG
3	D	144	GLU
3	D	147	VAL
3	D	150	LYS
3	D	164	VAL
3	D	171	ASP
3	D	173	THR
3	D	182	LEU
3	D	196	GLU
3	D	202	LEU
3	D	212	ARG
2	E	2	VAL
2	E	7	SER
2	E	54	TYR
2	E	67	ARG
2	E	81	LEU
2	E	89	GLU
2	E	99	ASP
2	E	102	MET
2	E	121	GLN
2	E	126	THR
2	E	132	THR
2	E	140	LEU
2	E	156	CYS
2	E	165	PRO
2	E	168	VAL
2	E	172	SER
2	E	175	LEU
2	E	195	SER
2	E	223	VAL
2	E	225	LYS
3	F	9	SER

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Mol	Chain	Res	Type
3	F	15	VAL
3	F	26	SER
3	F	31	SER
3	F	40	PRO
3	F	63	SER
3	F	70	ASP
3	F	92	SER
3	F	94	SER
3	F	95	PHE
3	F	98	THR
3	F	101	GLN
3	F	107	ILE
3	F	109	ARG
3	F	122	SER
3	F	123	ASP
3	F	132	SER
3	F	143	ARG
3	F	147	VAL
3	F	161	GLN
3	F	182	LEU
3	F	198	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	53	HIS
1	A	157	HIS
1	A	190	HIS
1	A	312	ASN
1	A	332	HIS
1	A	418	ASN
1	A	573	ASN
1	A	605	ASN
1	A	743	GLN
1	A	781	GLN
1	A	796	GLN
1	A	915	GLN
1	B	396	GLN
1	B	519	ASN
1	B	528	ASN
1	B	573	ASN

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Mol	Chain	Res	Type
1	B	638	GLN
1	B	743	GLN
1	B	781	GLN
1	B	796	GLN
1	B	979	ASN
2	C	39	GLN
2	C	121	GLN
3	D	167	GLN
2	E	39	GLN
2	E	215	ASN
2	E	216	HIS
3	F	90	GLN
3	F	161	GLN
3	F	167	GLN

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	932/990 (94%)	0.35	42 (4%)	38	27	12, 39, 101, 152	0
1	B	861/990 (86%)	0.35	43 (4%)	34	24	11, 41, 100, 151	0
2	C	216/263 (82%)	0.52	8 (3%)	45	32	19, 56, 97, 112	0
2	E	211/263 (80%)	0.61	13 (6%)	26	20	18, 55, 98, 144	0
3	D	199/239 (83%)	0.70	13 (6%)	25	18	22, 55, 102, 138	0
3	F	197/239 (82%)	0.58	9 (4%)	37	27	20, 69, 116, 147	0
All	All	2616/2984 (87%)	0.43	128 (4%)	35	25	11, 46, 103, 152	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	706	ASP	5.5
1	B	99	ASP	5.1
1	A	279	GLU	4.4
1	A	138	SER	4.1
1	A	507	ASP	4.0
1	B	241	LEU	3.9
1	B	59	GLU	3.8
1	A	798	ASP	3.7
1	B	325	TYR	3.6
2	E	22	CYS	3.6
1	A	458	GLU	3.5
1	B	378	ASP	3.5
3	D	162	GLU	3.4
1	A	182	GLU	3.4
1	B	174	PHE	3.4
1	B	370	PHE	3.4
3	F	179	THR	3.4
3	D	138	ASN	3.3
3	F	65	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	277	GLU	3.3
1	A	378	ASP	3.2
1	A	545	THR	3.2
3	D	88	CYS	3.1
1	B	173	LEU	3.1
3	F	135	CYS	3.1
2	C	70	ILE	3.1
3	D	50	SER	3.0
1	B	437	ILE	3.0
1	B	84	ASP	3.0
3	D	5	THR	3.0
1	A	413	GLU	3.0
3	F	88	CYS	3.0
2	E	121	GLN	2.9
1	B	321	ASP	2.9
1	B	45	PRO	2.9
1	A	137	SER	2.8
1	A	178	ALA	2.8
1	B	277	GLU	2.8
1	A	265	ASP	2.7
1	A	383	GLY	2.7
1	B	92	VAL	2.7
1	B	744	MET	2.7
2	E	110	TYR	2.7
2	C	46	GLU	2.6
1	A	116	LEU	2.6
2	E	106	SER	2.6
2	E	117	ASP	2.6
1	B	115	PHE	2.6
1	A	803	SER	2.5
2	E	99	ASP	2.5
1	A	227	GLU	2.5
1	B	879	GLU	2.5
1	B	47	ILE	2.5
1	A	84	ASP	2.5
1	B	310	ILE	2.5
2	C	65	LYS	2.5
1	B	371	MET	2.5
3	D	25	ALA	2.4
3	D	4	MET	2.4
1	A	542	LYS	2.4
1	B	448	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	768	GLU	2.4
1	B	457	GLU	2.4
2	E	85	SER	2.4
3	F	178	SER	2.4
1	A	174	PHE	2.4
2	E	107	PHE	2.4
1	A	627	MET	2.3
2	E	186	LEU	2.3
1	A	457	GLU	2.3
1	B	91	ASP	2.3
1	B	151	PHE	2.3
3	D	144	GLU	2.3
1	B	426	ASP	2.3
1	B	565	ASP	2.3
1	B	322	LEU	2.3
3	D	65	SER	2.3
3	F	63	SER	2.3
1	B	507	ASP	2.3
1	B	705	ASP	2.3
1	A	486	GLU	2.2
1	A	121	TYR	2.2
1	A	177	SER	2.2
3	F	195	CYS	2.2
1	A	133	GLU	2.2
1	B	113	MET	2.2
2	E	40	ALA	2.2
1	B	109	PHE	2.2
3	F	187	TYR	2.2
1	A	759	LEU	2.2
3	D	29	VAL	2.2
2	C	21	SER	2.2
2	C	193	SER	2.2
1	B	458	GLU	2.2
2	E	113	PRO	2.2
1	B	659	PHE	2.2
3	D	116	VAL	2.2
1	A	404	GLU	2.2
1	A	335	GLY	2.2
1	B	165	PHE	2.2
2	E	175	LEU	2.1
1	A	191	GLU	2.1
1	B	63	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLU	2.1
1	B	540	LEU	2.1
2	E	6	GLU	2.1
3	F	11	LEU	2.1
1	A	159	GLU	2.1
1	A	726	GLU	2.1
1	A	910	GLU	2.1
1	B	702	GLU	2.1
1	A	115	PHE	2.1
3	D	9	SER	2.1
2	C	156	CYS	2.1
2	C	22	CYS	2.1
1	A	173	LEU	2.0
1	A	416	ASP	2.0
1	B	876	ASP	2.0
1	A	656	GLU	2.0
1	A	241	LEU	2.0
1	A	171	SER	2.0
3	D	94	SER	2.0
1	A	516	ALA	2.0
2	C	130	ALA	2.0
1	A	91	ASP	2.0
1	A	244	PHE	2.0
1	B	982	GLN	2.0
1	B	726	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
4	ZN	A	1101	1/1	0.95	0.04	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.