



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:18 PM UTC

PDB ID : 4B3L / pdb_00004b3l
Title : Family 1 6-phospho-beta-D glycosidase from Streptococcus pyogenes
Authors : Stepper, J.; Dabin, J.; Ekloef, J.M.; Thongpoo, P.; Kongsaree, P.T.; Taylor, E.J.; Turkenburg, J.P.; Brumer, H.; Davies, G.J.
Deposited on : 2012-07-24
Resolution : 2.51 Å(reported)

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

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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

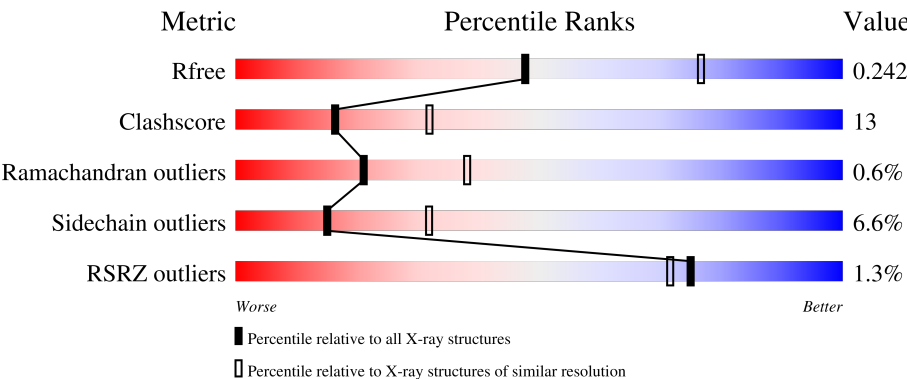
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	479	
1	B	479	
1	C	479	
1	D	479	
1	E	479	

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Mol	Chain	Length	Quality of chain
1	F	479	5% 55% 35% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22619 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 BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	B	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	C	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	D	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	E	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	F	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			

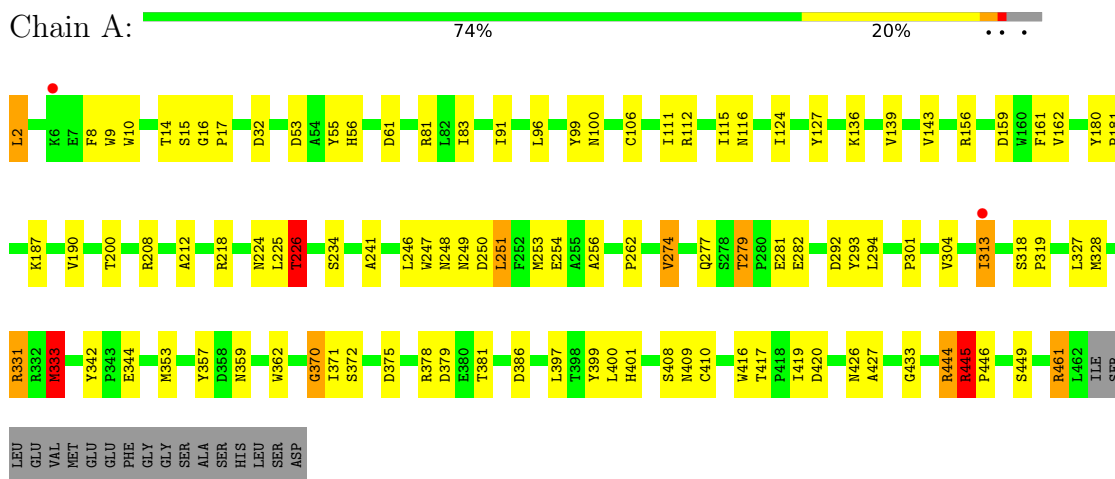
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	4	Total	O	0	0
			4	4		
2	C	3	Total	O	0	0
			3	3		
2	D	5	Total	O	0	0
			5	5		
2	E	1	Total	O	0	0
			1	1		
2	F	3	Total	O	0	0
			3	3		

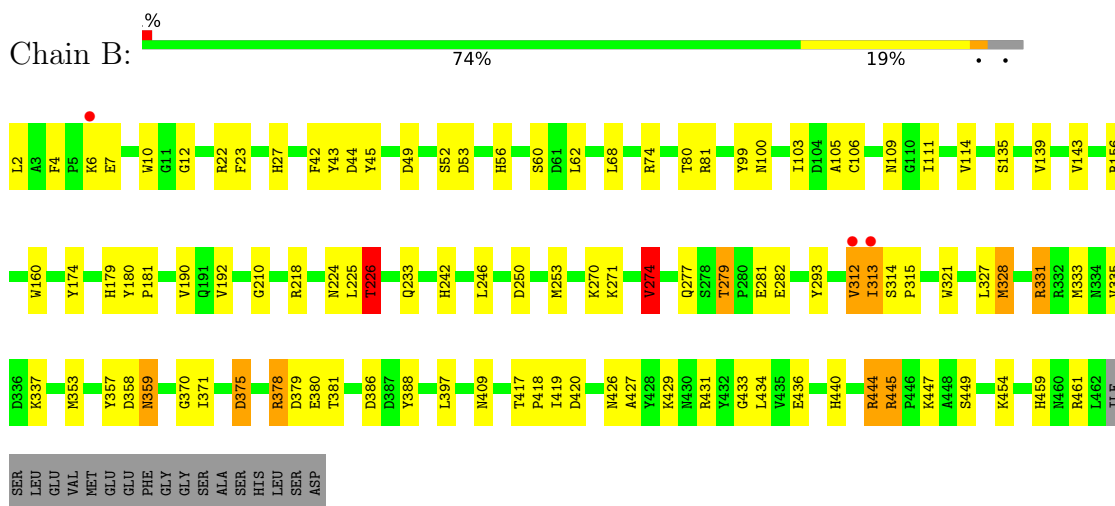
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: BETA-GLUCOSIDASE

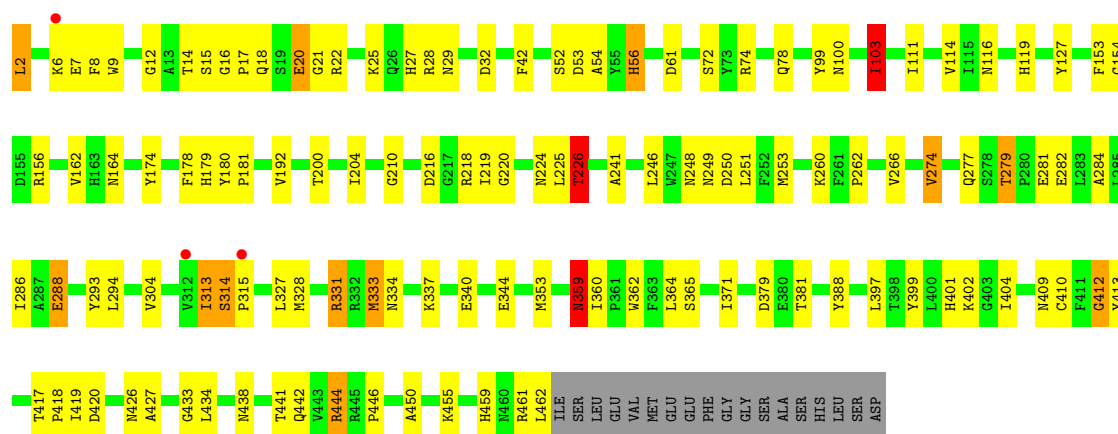


• Molecule 1: BETA-GLUCOSIDASE



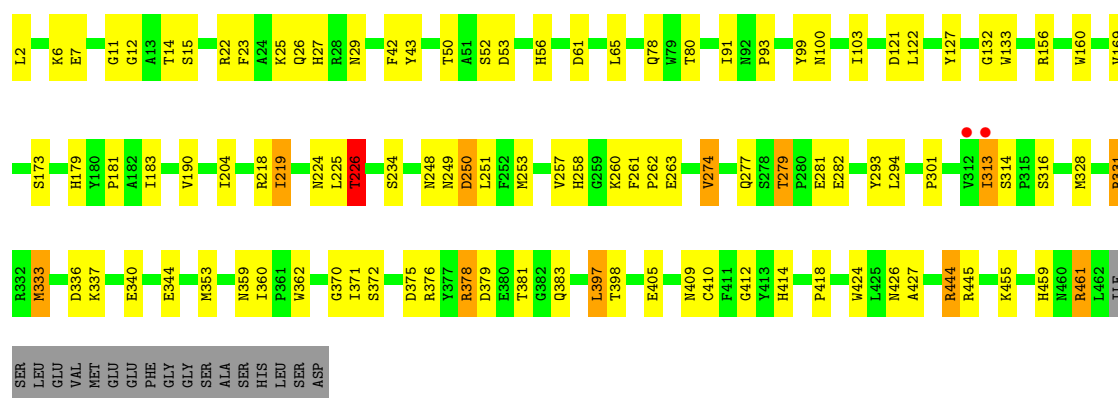
• Molecule 1: BETA-GLUCOSIDASE





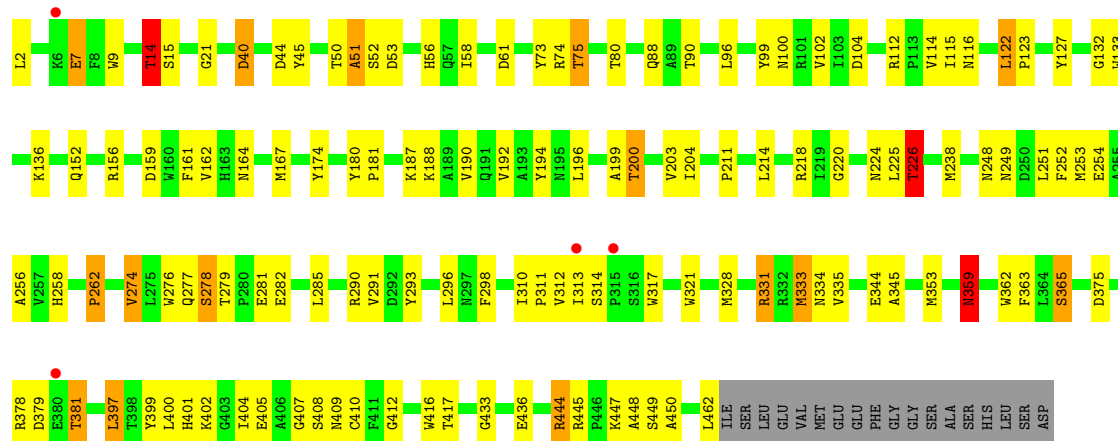
• Molecule 1: BETA-GLUCOSIDASE

Chain D: 74% 20%



• Molecule 1: BETA-GLUCOSIDASE

Chain E: 68% 24%



• Molecule 1: BETA-GLUCOSIDASE

Chain F: 55% 35% 6% 5%

L462	L2	A105	P181	L265	M353
ILE	K6	C106	A182	V268	Y357
SER	G11	L107	I183	L269	D358
LEU		A108	V184	K270	N359
GLU		N109	D185	K271	I360
VAL		R112	G186	D272	P361
MET		P113	K187	G273	W362
GLU		V114	A188	V274	F363
GLU		I115	A189	L275	L364
PHE		N116	Q190	W276	S365
GLY		Q191	Q191	Q277	E366
GLY		L117	V192	S278	
SER		A193	A193	T279	E374
ALA		H118	Y194	P280	D375
SER		H119	N195	E281	
HIS		F120	L196	E282	R378
LEU		D121	A197	L283	D379
SER		L122	A199	A284	E380
SER		P123	T200	L285	T381
ASP		Y127	A201	I286	G382
		Y130	K202	N289	I384
		G131	T204		
		G132	Q205	Y293	R389
		W133		L294	I390
		E134	R208	G295	
		S135	E209	L296	L393
		K136		N297	
		H137	I219	D308	L397
		V138	G220		E405
		V139	T221	V312	
		D140	I222	I313	N409
		L141	N223	S314	C410
		F142	N224	P315	F411
		V143	L225	S316	G412
		A144	T226	W317	Y413
		F145		S318	H414
		S146	Q233	P319	V415
		K147	S234	E320	W416
		F150		W321	T417
		F153	N238	Y322	P418
		R156	F243	Y323	I419
		V157	L246	D324	D420
		K158	W247	L327	G433
		D159	N248	M328	L434
		W160	N249		V435
		F161	D250	R331	E436
		V162	L251	M332	N437
		E165	F252	N334	N438
		P166	E254	V335	R444
		V170	V257	E340	R445
		Y174	F261	I341	P446
		Y180	E264	A350	K447

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.83Å 198.04Å 107.88Å 90.00° 118.51° 90.00°	Depositor
Resolution (Å)	94.75 – 2.51 94.75 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (94.75-2.51) 99.5 (94.75-2.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.205 , 0.261 (Not available) , 0.242	Depositor DCC
R_{free} test set	6762 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.023 for -h-l,k,h 0.023 for l,k,-h-l 0.032 for h,-k,-h-l 0.034 for -h-l,-k,l 0.087 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22619	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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

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	1.07	1/3891 (0.0%)	1.15	11/5304 (0.2%)
1	B	1.09	3/3891 (0.1%)	1.14	9/5304 (0.2%)
1	C	1.09	4/3891 (0.1%)	1.15	16/5304 (0.3%)
1	D	1.07	1/3891 (0.0%)	1.11	10/5304 (0.2%)
1	E	1.02	1/3891 (0.0%)	1.13	9/5304 (0.2%)
1	F	1.12	2/3891 (0.1%)	1.23	22/5304 (0.4%)
All	All	1.08	12/23346 (0.1%)	1.15	77/31824 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	14	THR	C-O	6.66	1.30	1.24
1	C	438	ASN	N-CA	-5.57	1.39	1.46
1	C	27	HIS	CG-ND1	-5.51	1.32	1.38
1	F	70	HIS	CG-CD2	5.47	1.41	1.35
1	C	42	PHE	CA-C	-5.25	1.46	1.52
1	A	370	GLY	CA-C	5.16	1.56	1.51
1	C	56	HIS	CE1-NE2	5.14	1.37	1.32
1	F	70	HIS	CA-C	-5.11	1.46	1.52
1	D	179	HIS	CG-CD2	5.10	1.41	1.35
1	B	179	HIS	CG-CD2	5.09	1.41	1.35
1	B	429	LYS	C-O	-5.06	1.18	1.24
1	B	440	HIS	CG-CD2	5.06	1.41	1.35

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	THR	CA-C-N	-10.26	110.26	120.31
1	C	226	THR	C-N-CA	-10.26	110.26	120.31
1	E	21	GLY	N-CA-C	-9.47	102.51	112.08
1	E	226	THR	CA-C-N	-8.99	111.13	120.03
1	E	226	THR	C-N-CA	-8.99	111.13	120.03
1	F	21	GLY	N-CA-C	-7.86	101.64	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	314	SER	CA-C-N	7.72	129.50	119.84
1	F	314	SER	C-N-CA	7.72	129.50	119.84
1	B	226	THR	CA-C-N	-7.63	112.47	120.03
1	B	226	THR	C-N-CA	-7.63	112.47	120.03
1	F	323	TYR	N-CA-C	7.13	119.40	108.07
1	A	445	ARG	CA-C-N	7.11	127.51	119.83
1	A	445	ARG	C-N-CA	7.11	127.51	119.83
1	C	32	ASP	N-CA-C	-7.04	103.53	111.07
1	F	415	VAL	CB-CA-C	-6.92	103.75	111.23
1	A	55	TYR	N-CA-C	-6.87	103.87	111.36
1	E	122	LEU	CA-C-N	-6.83	112.62	119.99
1	E	122	LEU	C-N-CA	-6.83	112.62	119.99
1	A	115	ILE	N-CA-C	6.76	117.58	108.11
1	C	20	GLU	N-CA-C	6.66	118.33	111.14
1	A	226	THR	CA-C-N	-6.60	113.50	120.03
1	A	226	THR	C-N-CA	-6.60	113.50	120.03
1	D	121	ASP	N-CA-C	6.50	119.20	110.88
1	D	360	ILE	CA-C-N	-6.50	113.25	120.14
1	D	360	ILE	C-N-CA	-6.50	113.25	120.14
1	E	335	VAL	N-CA-C	6.35	116.51	110.42
1	E	75	THR	N-CA-C	-6.33	99.89	108.24
1	F	223	LEU	N-CA-C	6.32	116.61	108.34
1	D	226	THR	CA-C-N	-6.31	114.12	120.31
1	D	226	THR	C-N-CA	-6.31	114.12	120.31
1	C	103	ILE	CB-CA-C	-6.28	103.94	111.97
1	D	412	GLY	N-CA-C	6.23	119.60	110.38
1	F	186	GLY	N-CA-C	6.21	120.19	112.73
1	F	312	VAL	CB-CA-C	-6.21	103.75	112.14
1	B	312	VAL	CA-C-N	-5.97	114.37	122.91
1	B	312	VAL	C-N-CA	-5.97	114.37	122.91
1	F	279	THR	CA-C-N	5.93	126.35	119.47
1	F	279	THR	C-N-CA	5.93	126.35	119.47
1	A	32	ASP	N-CA-C	-5.93	104.74	111.14
1	F	460	ASN	N-CA-C	5.88	119.77	112.24
1	C	434	LEU	N-CA-C	-5.84	105.04	111.82
1	A	461	ARG	N-CA-C	5.84	116.11	107.88
1	F	91	ILE	N-CA-C	5.78	117.18	109.37
1	F	293	TYR	N-CA-C	5.77	116.70	108.74
1	F	26	GLN	N-CA-C	5.74	118.03	111.02
1	C	210	GLY	CA-C-N	5.71	125.72	119.90
1	C	210	GLY	C-N-CA	5.71	125.72	119.90
1	B	4	PHE	CA-C-N	-5.68	113.75	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	PHE	C-N-CA	-5.68	113.75	120.11
1	C	274	VAL	CB-CA-C	5.50	116.55	110.62
1	A	372	SER	N-CA-C	5.48	120.64	113.30
1	F	192	VAL	N-CA-C	-5.47	105.04	110.62
1	E	40	ASP	N-CA-C	-5.45	106.47	113.01
1	D	333	MET	N-CA-C	5.42	118.28	108.69
1	C	153	PHE	N-CA-C	-5.40	107.70	114.56
1	C	360	ILE	CA-C-N	-5.39	114.40	119.85
1	C	360	ILE	C-N-CA	-5.39	114.40	119.85
1	F	75	THR	N-CA-C	-5.37	100.67	108.07
1	A	333	MET	N-CA-C	5.33	117.50	109.23
1	C	21	GLY	N-CA-C	-5.30	106.35	112.29
1	D	424	TRP	CB-CA-C	-5.29	110.50	116.63
1	B	160	TRP	N-CA-C	5.25	117.47	108.90
1	C	412	GLY	N-CA-C	5.25	118.37	110.18
1	C	450	ALA	CA-C-N	5.25	127.75	120.29
1	C	450	ALA	C-N-CA	5.25	127.75	120.29
1	B	335	VAL	N-CA-C	5.21	116.55	110.62
1	F	324	ASP	CA-C-N	5.13	125.13	119.90
1	F	324	ASP	C-N-CA	5.13	125.13	119.90
1	A	256	ALA	N-CA-C	5.11	116.93	111.36
1	F	170	VAL	CB-CA-C	-5.11	105.43	111.81
1	B	10	TRP	N-CA-C	-5.09	100.73	109.24
1	E	115	ILE	N-CA-C	5.04	115.30	107.78
1	F	335	VAL	N-CA-C	5.04	115.47	110.23
1	F	182	ALA	CA-C-N	-5.03	116.89	122.27
1	F	182	ALA	C-N-CA	-5.03	116.89	122.27
1	D	26	GLN	N-CA-C	5.01	116.82	111.36
1	D	250	ASP	N-CA-C	5.00	116.81	111.36

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	3767	0	3574	79	0
1	B	3767	0	3574	80	0
1	C	3767	0	3574	82	0
1	D	3767	0	3574	71	0
1	E	3767	0	3574	102	0
1	F	3767	0	3574	160	0
2	A	1	0	0	0	0
2	B	4	0	0	2	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
2	E	1	0	0	0	0
2	F	3	0	0	0	0
All	All	22619	0	21444	571	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 13.

All (571) 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:224:ASN:OD1	1:B:226:THR:HG23	1.35	1.23
1:F:331:ARG:HH11	1:F:331:ARG:CG	1.47	1.22
1:B:331:ARG:CG	1:B:331:ARG:HH11	1.54	1.16
1:A:224:ASN:OD1	1:A:226:THR:HG23	1.46	1.16
1:F:331:ARG:HH11	1:F:331:ARG:HG2	1.10	1.15
1:C:224:ASN:OD1	1:C:226:THR:HG23	1.48	1.13
1:E:331:ARG:HG2	1:E:331:ARG:HH11	1.09	1.13
1:A:331:ARG:HH11	1:A:331:ARG:CG	1.63	1.11
1:E:112:ARG:HD3	1:E:159:ASP:OD2	1.54	1.07
1:E:224:ASN:OD1	1:E:226:THR:HG23	1.56	1.05
1:E:331:ARG:HH11	1:E:331:ARG:CG	1.69	1.04
1:A:331:ARG:HH11	1:A:331:ARG:HG2	0.91	1.04
1:B:331:ARG:HH11	1:B:331:ARG:HG3	1.23	1.03
1:F:81:ARG:HG3	1:F:81:ARG:HH11	1.21	1.01
1:F:359:ASN:HD21	1:F:409:ASN:H	1.06	0.98
1:C:379:ASP:OD1	1:C:381:THR:HG22	1.64	0.96
1:A:331:ARG:HG2	1:A:331:ARG:NH1	1.72	0.96
1:B:224:ASN:OD1	1:B:226:THR:CG2	2.13	0.95
1:A:253:MET:CE	1:A:353:MET:HE1	1.95	0.95
1:C:225:LEU:HD22	1:C:353:MET:HE3	1.49	0.95
1:F:199:ALA:O	1:F:203:VAL:HG23	1.67	0.94
1:F:331:ARG:CG	1:F:331:ARG:NH1	2.21	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASN:OD1	1:F:226:THR:HG23	1.68	0.92
1:C:225:LEU:CD2	1:C:353:MET:HE3	2.00	0.91
1:D:331:ARG:HH11	1:D:331:ARG:HG2	1.35	0.91
1:A:379:ASP:OD1	1:A:381:THR:HG22	1.70	0.91
1:E:282:GLU:HA	1:E:285:LEU:HD12	1.52	0.91
1:D:353:MET:HE2	1:D:353:MET:HA	1.52	0.90
1:B:331:ARG:HH11	1:B:331:ARG:HG2	1.34	0.90
1:F:331:ARG:HG2	1:F:331:ARG:NH1	1.79	0.90
1:F:331:ARG:HH11	1:F:331:ARG:HG3	1.35	0.89
1:B:331:ARG:CG	1:B:331:ARG:NH1	2.26	0.89
1:E:136:LYS:HZ3	1:E:194:TYR:HE2	1.13	0.88
1:C:328:MET:O	1:C:331:ARG:HD3	1.75	0.87
1:E:188:LYS:O	1:E:192:VAL:HG23	1.74	0.86
1:C:174:TYR:CE2	1:C:192:VAL:HG21	2.11	0.85
1:B:100:ASN:ND2	1:B:156:ARG:HH22	1.75	0.85
1:A:253:MET:HE1	1:A:353:MET:HE1	1.60	0.83
1:B:279:THR:HG22	1:B:282:GLU:H	1.44	0.82
1:E:52:SER:O	1:E:444:ARG:NH2	2.13	0.81
1:F:297:ASN:ND2	1:F:366:GLU:HB2	1.95	0.81
1:A:253:MET:HE2	1:A:353:MET:HE1	1.62	0.81
1:F:160:TRP:HB2	1:F:219:ILE:CG2	2.11	0.81
1:B:100:ASN:HD21	1:B:156:ARG:HH22	1.23	0.81
1:F:122:LEU:HD12	1:F:123:PRO:HD2	1.63	0.80
1:D:279:THR:HG22	1:D:282:GLU:H	1.47	0.80
1:B:225:LEU:HD22	1:B:353:MET:HE3	1.61	0.80
1:B:445:ARG:HH11	1:B:445:ARG:CG	1.94	0.80
1:A:224:ASN:OD1	1:A:226:THR:CG2	2.28	0.79
1:D:53:ASP:OD1	1:D:56:HIS:HD2	1.66	0.79
1:F:112:ARG:HD3	1:F:159:ASP:OD2	1.82	0.79
1:F:81:ARG:HG3	1:F:81:ARG:NH1	1.96	0.78
1:B:445:ARG:HH11	1:B:445:ARG:HG3	1.49	0.77
1:E:254:GLU:HG3	1:E:262:PRO:HG3	1.65	0.77
1:B:359:ASN:HD21	1:B:409:ASN:H	1.32	0.76
1:C:100:ASN:HD22	1:C:156:ARG:HH12	1.32	0.76
1:D:224:ASN:OD1	1:D:226:THR:CG2	2.34	0.75
1:C:224:ASN:OD1	1:C:226:THR:CG2	2.33	0.75
1:A:190:VAL:HG21	1:A:274:VAL:CG1	2.16	0.75
1:B:242:HIS:ND1	2:B:2003:HOH:O	1.83	0.75
1:D:359:ASN:HD21	1:D:409:ASN:H	1.30	0.75
1:F:160:TRP:HB2	1:F:219:ILE:HG22	1.70	0.74
1:C:100:ASN:ND2	1:C:156:ARG:HH12	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD22	1:A:353:MET:HE3	1.70	0.74
1:F:61:ASP:OD1	1:F:444:ARG:NH1	2.21	0.74
1:D:331:ARG:NH1	1:D:333:MET:HB2	2.02	0.74
1:F:162:VAL:HG21	1:F:200:THR:HG23	1.70	0.72
1:C:53:ASP:OD1	1:C:56:HIS:HD2	1.73	0.72
1:D:331:ARG:HH12	1:D:333:MET:HB2	1.53	0.71
1:D:331:ARG:HG2	1:D:331:ARG:NH1	2.03	0.71
1:F:26:GLN:OE1	1:F:92:ASN:ND2	2.23	0.71
1:B:44:ASP:O	1:B:45:TYR:HB2	1.88	0.71
1:B:331:ARG:HG3	1:B:331:ARG:NH1	1.99	0.71
1:A:331:ARG:CG	1:A:331:ARG:NH1	2.35	0.71
1:F:74:ARG:HA	1:F:114:VAL:O	1.90	0.71
1:F:353:MET:HE2	1:F:353:MET:HA	1.72	0.71
1:E:331:ARG:CG	1:E:331:ARG:NH1	2.37	0.71
1:D:224:ASN:OD1	1:D:226:THR:HG22	1.91	0.70
1:B:434:LEU:O	1:B:447:LYS:HG3	1.91	0.70
1:F:15:SER:O	1:F:19:SER:OG	2.08	0.70
1:F:277:GLN:HA	1:F:277:GLN:NE2	2.06	0.70
1:F:275:LEU:HD12	1:F:276:TRP:H	1.56	0.69
1:F:225:LEU:HD13	1:F:253:MET:HG3	1.74	0.69
1:F:52:SER:O	1:F:444:ARG:NH2	2.25	0.69
1:B:279:THR:CG2	1:B:281:GLU:HB2	2.22	0.69
1:B:331:ARG:HG2	1:B:331:ARG:NH1	1.97	0.69
1:E:100:ASN:HD21	1:E:156:ARG:HH22	1.39	0.69
1:B:53:ASP:OD1	1:B:56:HIS:HD2	1.76	0.69
1:E:381:THR:HG23	1:E:445:ARG:NH2	2.08	0.68
1:D:379:ASP:OD1	1:D:381:THR:CG2	2.41	0.68
1:C:459:HIS:O	1:C:461:ARG:HG3	1.93	0.68
1:D:160:TRP:HB2	1:D:219:ILE:HG13	1.76	0.68
1:F:188:LYS:O	1:F:192:VAL:HG23	1.93	0.68
1:F:359:ASN:HD21	1:F:409:ASN:N	1.86	0.68
1:F:190:VAL:O	1:F:193:ALA:HB3	1.94	0.68
1:A:127:TYR:CZ	1:A:181:PRO:HG3	2.28	0.68
1:A:61:ASP:OD1	1:A:444:ARG:HD2	1.94	0.67
1:C:417:THR:O	1:C:433:GLY:HA2	1.94	0.67
1:A:253:MET:HE2	1:A:353:MET:CE	2.24	0.67
1:A:359:ASN:HD21	1:A:408:SER:HA	1.59	0.67
1:E:328:MET:O	1:E:331:ARG:HD2	1.94	0.66
1:B:328:MET:O	1:B:331:ARG:HD2	1.96	0.66
1:E:194:TYR:CZ	1:E:278:SER:HB2	2.31	0.66
1:E:225:LEU:HD22	1:E:353:MET:CE	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:SER:O	1:F:238:MET:HB2	1.94	0.66
1:A:328:MET:O	1:A:331:ARG:HD2	1.96	0.66
1:A:139:VAL:O	1:A:143:VAL:HG23	1.96	0.66
1:C:225:LEU:CD2	1:C:353:MET:CE	2.73	0.66
1:C:25:LYS:NZ	1:C:78:GLN:HE22	1.94	0.65
1:E:359:ASN:HD21	1:E:409:ASN:H	1.44	0.65
1:B:105:ALA:O	1:B:109:ASN:ND2	2.24	0.65
1:E:14:THR:OG1	1:E:15:SER:N	2.28	0.65
1:E:225:LEU:HD22	1:E:353:MET:HE3	1.79	0.65
1:E:104:ASP:OD1	1:E:156:ARG:NH1	2.29	0.65
1:F:80:THR:HG23	1:F:123:PRO:HG3	1.79	0.65
1:F:87:GLU:OE2	1:F:130:TYR:OH	2.15	0.64
1:E:331:ARG:HG2	1:E:331:ARG:NH1	1.92	0.64
1:F:160:TRP:HB2	1:F:219:ILE:HG23	1.79	0.64
1:D:100:ASN:ND2	1:D:156:ARG:HH12	1.95	0.64
1:C:359:ASN:HD21	1:C:409:ASN:H	1.44	0.64
1:E:253:MET:CE	1:E:353:MET:HE1	2.28	0.64
1:F:105:ALA:O	1:F:109:ASN:HB2	1.98	0.64
1:E:56:HIS:CD2	1:F:56:HIS:CD2	2.86	0.64
1:F:58:ILE:HG12	1:F:102:VAL:HG22	1.79	0.64
1:C:2:LEU:HG	1:C:401:HIS:CE1	2.33	0.63
1:B:331:ARG:H	1:B:331:ARG:HD3	1.62	0.63
1:F:204:ILE:HG23	1:F:219:ILE:CD1	2.28	0.63
1:B:378:ARG:HH22	1:B:436:GLU:CD	2.06	0.63
1:C:251:LEU:C	1:C:251:LEU:HD23	2.24	0.63
1:D:225:LEU:CD2	1:D:353:MET:HE3	2.29	0.63
1:D:225:LEU:HD22	1:D:353:MET:HE3	1.80	0.63
1:D:379:ASP:OD1	1:D:381:THR:HG23	1.98	0.63
1:E:379:ASP:OD1	1:E:381:THR:HG22	1.99	0.63
1:C:253:MET:HE1	1:C:353:MET:HE1	1.80	0.63
1:F:275:LEU:HD12	1:F:276:TRP:N	2.14	0.63
1:B:253:MET:HE1	1:B:353:MET:HE1	1.79	0.62
1:F:378:ARG:HH22	1:F:436:GLU:CD	2.06	0.62
1:B:253:MET:CE	1:B:353:MET:HE1	2.29	0.62
1:A:53:ASP:OD1	1:A:56:HIS:HD2	1.83	0.62
1:D:99:TYR:O	1:D:103:ILE:HG12	2.00	0.62
1:F:103:ILE:HD13	1:F:103:ILE:N	2.15	0.62
1:E:174:TYR:CE2	1:E:192:VAL:HG21	2.34	0.62
1:E:100:ASN:ND2	1:E:156:ARG:HH22	1.98	0.62
1:F:84:ASP:HB3	1:F:90:THR:OG1	1.99	0.61
1:C:2:LEU:HG	1:C:401:HIS:ND1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:MET:CE	1:C:353:MET:HE1	2.30	0.61
1:E:296:LEU:HD11	1:E:353:MET:HE3	1.82	0.61
1:D:375:ASP:OD1	1:D:378:ARG:HD2	2.00	0.61
1:C:6:LYS:O	1:C:7:GLU:HB2	2.01	0.61
1:E:258:HIS:HA	1:E:290:ARG:NH1	2.16	0.61
1:B:174:TYR:CE2	1:B:192:VAL:HG21	2.35	0.61
1:E:251:LEU:C	1:E:251:LEU:HD23	2.24	0.61
1:F:11:GLY:HA2	1:F:70:HIS:ND1	2.14	0.61
1:F:277:GLN:HA	1:F:277:GLN:HE21	1.62	0.61
1:D:169:VAL:O	1:D:173:SER:HB2	2.00	0.61
1:B:225:LEU:HD13	1:B:253:MET:HG3	1.83	0.61
1:A:379:ASP:CG	1:A:381:THR:HG22	2.26	0.61
1:F:205:GLN:HB2	1:F:289:ASN:ND2	2.16	0.61
1:F:208:ARG:NH2	1:F:219:ILE:HD11	2.15	0.61
1:B:445:ARG:HG3	1:B:445:ARG:NH1	2.16	0.60
1:F:58:ILE:O	1:F:61:ASP:HB2	2.00	0.60
1:D:53:ASP:OD1	1:D:56:HIS:CD2	2.53	0.60
1:D:362:TRP:O	1:D:410:CYS:HA	2.00	0.60
1:A:279:THR:HG22	1:A:282:GLU:H	1.67	0.60
1:A:112:ARG:HD3	1:A:159:ASP:OD2	2.00	0.60
1:C:331:ARG:HG3	1:C:340:GLU:HG3	1.82	0.60
1:F:219:ILE:HD12	1:F:219:ILE:O	2.02	0.59
1:F:81:ARG:HH11	1:F:81:ARG:CG	2.07	0.59
1:F:143:VAL:O	1:F:146:SER:OG	2.16	0.59
1:F:359:ASN:ND2	1:F:409:ASN:H	1.88	0.59
1:A:375:ASP:O	1:A:378:ARG:HG3	2.01	0.59
1:B:328:MET:O	1:B:331:ARG:CD	2.50	0.59
1:E:220:GLY:HA2	1:E:291:VAL:HG12	1.84	0.59
1:A:208:ARG:HH21	1:A:292:ASP:CG	2.10	0.59
1:A:253:MET:CE	1:A:353:MET:CE	2.77	0.59
1:E:167:MET:HE2	1:E:252:PHE:HE2	1.67	0.59
1:F:59:GLU:OE2	1:F:101:ARG:HB3	2.02	0.59
1:C:246:LEU:HA	1:C:250:ASP:HB2	1.85	0.58
1:A:136:LYS:NZ	1:A:282:GLU:OE1	2.34	0.58
1:F:435:VAL:HG13	1:F:445:ARG:C	2.28	0.58
1:B:100:ASN:HD22	1:B:156:ARG:HH12	1.51	0.58
1:C:99:TYR:O	1:C:103:ILE:HG12	2.04	0.58
1:D:224:ASN:OD1	1:D:226:THR:HG23	2.03	0.58
1:E:133:TRP:HB2	1:E:192:VAL:HG13	1.86	0.58
1:E:279:THR:HG22	1:E:281:GLU:H	1.69	0.58
1:B:314:SER:HB2	1:B:321:TRP:CZ2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ASP:CG	1:C:381:THR:HG22	2.29	0.58
1:D:379:ASP:OD1	1:D:381:THR:HG22	2.04	0.58
1:E:167:MET:HE2	1:E:252:PHE:CE2	2.39	0.58
1:D:331:ARG:NH1	1:D:331:ARG:CG	2.67	0.57
1:F:264:GLU:O	1:F:268:VAL:HG23	2.04	0.57
1:C:419:ILE:HD13	1:C:444:ARG:HD3	1.86	0.57
1:C:251:LEU:HD23	1:C:251:LEU:O	2.04	0.57
1:E:74:ARG:HA	1:E:114:VAL:O	2.05	0.57
1:C:353:MET:HE2	1:C:353:MET:HA	1.87	0.57
1:D:100:ASN:HD22	1:D:156:ARG:HH12	1.52	0.57
1:C:74:ARG:HB2	1:C:114:VAL:HB	1.86	0.57
1:F:162:VAL:HG23	1:F:221:THR:HG22	1.87	0.57
1:F:251:LEU:HD23	1:F:251:LEU:C	2.29	0.57
1:A:251:LEU:HD23	1:A:251:LEU:O	2.05	0.56
1:E:194:TYR:OH	1:E:278:SER:HB2	2.06	0.56
1:A:331:ARG:HH12	1:A:333:MET:HB3	1.70	0.56
1:A:190:VAL:HG21	1:A:274:VAL:HG13	1.87	0.56
1:E:417:THR:O	1:E:433:GLY:HA2	2.06	0.56
1:F:365:SER:O	1:F:414:HIS:HB2	2.06	0.56
1:B:379:ASP:OD1	1:B:381:THR:HG22	2.06	0.56
1:F:204:ILE:HG23	1:F:219:ILE:HD13	1.87	0.56
1:F:363:PHE:HB2	1:F:412:GLY:O	2.06	0.56
1:F:435:VAL:HG22	1:F:446:PRO:HA	1.87	0.56
1:F:103:ILE:O	1:F:106:CYS:HB2	2.06	0.55
1:B:44:ASP:O	1:B:45:TYR:CB	2.51	0.55
1:F:331:ARG:NH1	1:F:331:ARG:HG3	2.04	0.55
1:B:314:SER:HB2	1:B:321:TRP:HZ2	1.72	0.55
1:F:116:ASN:ND2	1:F:118:HIS:O	2.31	0.55
1:D:190:VAL:HG21	1:D:274:VAL:HG13	1.88	0.55
1:A:2:LEU:HG	1:A:401:HIS:ND1	2.21	0.55
1:F:246:LEU:HD13	1:F:265:LEU:HB2	1.88	0.55
1:F:248:ASN:C	1:F:249:ASN:HD22	2.15	0.55
1:F:360:ILE:HD12	1:F:361:PRO:O	2.07	0.55
1:C:225:LEU:HD13	1:C:253:MET:HG3	1.88	0.55
1:C:362:TRP:O	1:C:410:CYS:HA	2.07	0.55
1:E:122:LEU:HD21	1:E:132:GLY:HA2	1.88	0.55
1:A:328:MET:O	1:A:331:ARG:CD	2.55	0.55
1:C:294:LEU:O	1:C:362:TRP:HA	2.07	0.55
1:E:253:MET:HE1	1:E:353:MET:HE1	1.88	0.55
1:B:426:ASN:O	1:B:427:ALA:C	2.49	0.54
1:F:357:TYR:O	1:F:360:ILE:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:GLY:O	1:D:371:ILE:HD13	2.07	0.54
1:C:248:ASN:C	1:C:249:ASN:HD22	2.15	0.54
1:C:251:LEU:C	1:C:251:LEU:CD2	2.80	0.54
1:E:362:TRP:O	1:E:410:CYS:HA	2.08	0.54
1:A:344:GLU:HG3	1:A:399:TYR:CZ	2.42	0.54
1:B:81:ARG:HD2	1:B:99:TYR:CE2	2.43	0.54
1:C:61:ASP:OD1	1:C:444:ARG:HD2	2.06	0.54
1:E:61:ASP:OD1	1:E:444:ARG:HD2	2.07	0.54
1:F:146:SER:HB2	1:F:150:PHE:CE2	2.43	0.54
1:D:328:MET:O	1:D:331:ARG:HD2	2.08	0.54
1:F:378:ARG:NH2	1:F:436:GLU:OE1	2.41	0.54
1:A:331:ARG:HD3	1:A:331:ARG:H	1.74	0.53
1:F:160:TRP:CB	1:F:219:ILE:HG22	2.36	0.53
1:F:222:ILE:HA	1:F:295:GLY:O	2.08	0.53
1:F:317:TRP:HD1	1:F:321:TRP:CZ3	2.26	0.53
1:D:279:THR:HG23	1:D:281:GLU:OE1	2.09	0.53
1:F:104:ASP:OD1	1:F:156:ARG:NH1	2.31	0.53
1:A:251:LEU:HD23	1:A:251:LEU:C	2.33	0.53
1:D:353:MET:HA	1:D:353:MET:CE	2.28	0.53
1:C:22:ARG:NH2	1:C:28:ARG:HG2	2.24	0.53
1:F:27:HIS:HB2	1:F:80:THR:HB	1.89	0.53
1:F:99:TYR:HB2	1:F:153:PHE:CZ	2.43	0.53
1:F:374:GLU:OE1	1:F:447:LYS:NZ	2.40	0.53
1:B:386:ASP:OD2	1:B:449:SER:OG	2.26	0.53
1:C:12:GLY:HA3	1:C:418:PRO:HG3	1.91	0.53
1:C:284:ALA:O	1:C:288:GLU:HB2	2.08	0.53
1:F:116:ASN:HA	1:F:161:PHE:O	2.09	0.53
1:D:378:ARG:HA	1:D:383:GLN:O	2.09	0.52
1:F:225:LEU:HD12	1:F:249:ASN:HB3	1.91	0.52
1:F:417:THR:O	1:F:433:GLY:HA2	2.10	0.52
1:E:56:HIS:CD2	1:F:56:HIS:NE2	2.77	0.52
1:E:256:ALA:O	1:E:291:VAL:HG22	2.09	0.52
1:F:139:VAL:HG13	1:F:199:ALA:HB2	1.92	0.52
1:B:370:GLY:HA2	1:B:431:ARG:O	2.09	0.52
1:D:42:PHE:O	1:D:43:TYR:C	2.52	0.52
1:C:333:MET:HG3	1:C:334:ASN:N	2.25	0.52
1:F:25:LYS:NZ	1:F:78:GLN:HE22	2.07	0.52
1:A:106:CYS:HB3	1:A:111:ILE:O	2.10	0.51
1:F:362:TRP:O	1:F:410:CYS:HA	2.11	0.51
1:E:196:LEU:O	1:E:200:THR:OG1	2.28	0.51
1:F:384:ILE:HB	1:F:447:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:HIS:O	1:D:461:ARG:HG2	2.11	0.51
1:E:50:THR:O	1:E:51:ALA:C	2.53	0.51
1:E:381:THR:HG23	1:E:445:ARG:HH22	1.75	0.51
1:F:204:ILE:HD12	1:F:219:ILE:HB	1.91	0.51
1:D:91:ILE:O	1:D:93:PRO:HD3	2.10	0.51
1:A:419:ILE:O	1:A:420:ASP:C	2.53	0.51
1:F:29:ASN:HD22	1:F:78:GLN:NE2	2.08	0.51
1:F:100:ASN:ND2	1:F:156:ARG:HH22	2.08	0.51
1:A:208:ARG:NH2	1:A:292:ASP:OD1	2.43	0.51
1:C:225:LEU:HD22	1:C:353:MET:CE	2.30	0.51
1:E:397:LEU:O	1:E:400:LEU:HB3	2.11	0.51
1:B:357:TYR:C	1:B:359:ASN:H	2.20	0.50
1:D:6:LYS:O	1:D:7:GLU:HB2	2.10	0.50
1:E:53:ASP:OD1	1:E:56:HIS:HD2	1.92	0.50
1:F:15:SER:HB3	1:F:119:HIS:CD2	2.47	0.50
1:F:174:TYR:CE2	1:F:192:VAL:HG21	2.47	0.50
1:A:294:LEU:O	1:A:362:TRP:HA	2.11	0.50
1:A:53:ASP:OD1	1:A:56:HIS:CD2	2.65	0.50
1:F:378:ARG:HA	1:F:383:GLN:O	2.11	0.50
1:A:331:ARG:HH12	1:A:333:MET:CB	2.24	0.50
1:A:370:GLY:O	1:A:371:ILE:HD13	2.12	0.50
1:B:379:ASP:OD1	1:B:381:THR:CG2	2.60	0.50
1:E:253:MET:HE2	1:E:353:MET:HE1	1.91	0.50
1:F:16:GLY:N	1:F:17:PRO:CD	2.75	0.50
1:D:344:GLU:CD	1:D:344:GLU:H	2.19	0.50
1:E:248:ASN:C	1:E:249:ASN:HD22	2.20	0.50
1:E:331:ARG:NH1	1:E:333:MET:HB2	2.27	0.50
1:F:251:LEU:HD12	1:F:265:LEU:HD21	1.91	0.50
1:A:251:LEU:C	1:A:251:LEU:CD2	2.85	0.50
1:A:379:ASP:OD1	1:A:381:THR:CG2	2.51	0.50
1:F:161:PHE:HD2	1:F:221:THR:N	2.10	0.50
1:E:74:ARG:NH2	1:E:164:ASN:OD1	2.44	0.49
1:E:180:TYR:CG	1:E:181:PRO:HA	2.48	0.49
1:F:297:ASN:HD22	1:F:366:GLU:H	1.59	0.49
1:A:331:ARG:NH1	1:A:333:MET:HB3	2.26	0.49
1:C:25:LYS:HZ3	1:C:78:GLN:HE22	1.60	0.49
1:A:386:ASP:OD2	1:A:449:SER:HB3	2.12	0.49
1:D:6:LYS:O	1:D:7:GLU:CB	2.61	0.49
1:E:200:THR:O	1:E:204:ILE:HG12	2.13	0.49
1:F:297:ASN:HD22	1:F:366:GLU:N	2.11	0.49
1:A:127:TYR:CE1	1:A:181:PRO:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:HIS:CD2	1:F:141:LEU:HD11	2.48	0.49
1:E:80:THR:HG22	1:E:123:PRO:HB3	1.95	0.48
1:E:190:VAL:HG21	1:E:274:VAL:HG22	1.94	0.48
1:A:241:ALA:HA	1:A:304:VAL:HG21	1.96	0.48
1:C:127:TYR:CZ	1:C:181:PRO:HG3	2.48	0.48
1:E:96:LEU:HD11	1:E:152:GLN:HE21	1.78	0.48
1:E:344:GLU:HG3	1:E:399:TYR:CZ	2.48	0.48
1:F:268:VAL:O	1:F:272:ASP:OD1	2.31	0.48
1:A:417:THR:O	1:A:433:GLY:HA2	2.13	0.48
1:F:366:GLU:HG2	1:F:416:TRP:HE3	1.77	0.48
1:B:419:ILE:O	1:B:420:ASP:C	2.55	0.48
1:D:100:ASN:HD21	1:D:156:ARG:HH22	1.60	0.48
1:F:130:TYR:CE2	1:F:137:HIS:HD2	2.30	0.48
1:F:201:ALA:HB2	1:F:286:ILE:HA	1.95	0.48
1:A:8:PHE:HD2	1:A:10:TRP:CE2	2.31	0.48
1:B:99:TYR:O	1:B:103:ILE:HG12	2.14	0.48
1:B:100:ASN:ND2	1:B:156:ARG:NH2	2.54	0.48
1:F:419:ILE:O	1:F:420:ASP:C	2.57	0.48
1:D:257:VAL:HG12	1:D:258:HIS:CD2	2.49	0.48
1:E:187:LYS:HA	1:E:274:VAL:HG23	1.95	0.48
1:E:375:ASP:OD1	1:E:378:ARG:NH1	2.46	0.48
1:F:317:TRP:HA	1:F:321:TRP:CZ2	2.49	0.48
1:A:100:ASN:ND2	1:A:156:ARG:HH22	2.12	0.48
1:B:246:LEU:HA	1:B:250:ASP:HB2	1.96	0.48
1:F:383:GLN:HG2	1:F:384:ILE:N	2.29	0.48
1:F:397:LEU:HB3	1:F:462:LEU:HD11	1.96	0.48
1:E:56:HIS:NE2	1:F:56:HIS:CD2	2.82	0.48
1:F:133:TRP:O	1:F:192:VAL:HG22	2.14	0.48
1:B:52:SER:O	1:B:444:ARG:NH2	2.40	0.47
1:C:6:LYS:O	1:C:7:GLU:CB	2.62	0.47
1:F:29:ASN:HD22	1:F:78:GLN:HE21	1.61	0.47
1:A:353:MET:HE2	1:A:357:TYR:CD2	2.49	0.47
1:C:344:GLU:HG3	1:C:399:TYR:CZ	2.49	0.47
1:C:371:ILE:HG13	1:C:388:TYR:CE1	2.48	0.47
1:E:9:TRP:HB2	1:E:412:GLY:HA3	1.96	0.47
1:F:205:GLN:OE1	1:F:285:LEU:CD2	2.61	0.47
1:A:91:ILE:HG21	1:A:96:LEU:HD22	1.96	0.47
1:D:11:GLY:O	1:D:414:HIS:HA	2.15	0.47
1:C:20:GLU:HA	1:C:54:ALA:HB3	1.95	0.47
1:C:279:THR:HG22	1:C:282:GLU:H	1.78	0.47
1:C:362:TRP:CZ2	1:C:410:CYS:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:THR:OG1	1:D:15:SER:N	2.47	0.47
1:D:6:LYS:C	1:D:7:GLU:HG2	2.40	0.47
1:D:127:TYR:HA	1:D:132:GLY:N	2.29	0.47
1:E:331:ARG:NH1	1:E:331:ARG:HG3	2.24	0.47
1:F:122:LEU:HD12	1:F:123:PRO:CD	2.38	0.47
1:B:378:ARG:NH2	1:B:436:GLU:OE1	2.47	0.47
1:C:401:HIS:O	1:C:404:ILE:N	2.47	0.47
1:F:136:LYS:O	1:F:139:VAL:HB	2.14	0.47
1:F:201:ALA:CB	1:F:286:ILE:HA	2.45	0.47
1:B:379:ASP:CG	1:B:381:THR:HG22	2.40	0.47
1:C:162:VAL:HG11	1:C:200:THR:HA	1.97	0.47
1:E:61:ASP:CG	1:E:444:ARG:HH11	2.23	0.47
1:E:133:TRP:CB	1:E:192:VAL:HG13	2.45	0.47
1:E:416:TRP:CD1	1:E:417:THR:HB	2.50	0.47
1:A:444:ARG:H	1:A:444:ARG:HG2	1.54	0.47
1:A:162:VAL:HG11	1:A:200:THR:HA	1.95	0.46
1:D:25:LYS:NZ	1:D:78:GLN:HE22	2.12	0.46
1:F:314:SER:HA	1:F:315:PRO:HD2	1.65	0.46
1:B:313:ILE:HD12	1:B:314:SER:H	1.80	0.46
1:C:279:THR:HG23	1:C:281:GLU:OE1	2.16	0.46
1:E:127:TYR:HA	1:E:132:GLY:N	2.31	0.46
1:B:314:SER:O	1:B:315:PRO:C	2.57	0.46
1:C:241:ALA:HA	1:C:304:VAL:HG21	1.97	0.46
1:D:127:TYR:CZ	1:D:181:PRO:HG3	2.50	0.46
1:E:211:PRO:HG2	1:E:214:LEU:HD12	1.98	0.46
1:F:81:ARG:O	1:F:81:ARG:HG2	2.16	0.46
1:F:362:TRP:CE2	1:F:410:CYS:HB2	2.51	0.46
1:D:29:ASN:HD22	1:D:78:GLN:NE2	2.14	0.46
1:C:200:THR:O	1:C:204:ILE:HG13	2.15	0.46
1:B:279:THR:HG22	1:B:282:GLU:N	2.21	0.46
1:F:78:GLN:O	1:F:79:TRP:C	2.56	0.46
1:F:208:ARG:HH21	1:F:219:ILE:HD11	1.80	0.46
1:E:401:HIS:O	1:E:402:LYS:C	2.57	0.46
1:F:243:PHE:O	1:F:246:LEU:HB2	2.15	0.46
1:B:459:HIS:O	1:B:461:ARG:HG3	2.16	0.46
1:E:88:GLN:HB2	1:E:90:THR:HG23	1.97	0.46
1:F:127:TYR:HA	1:F:132:GLY:N	2.31	0.46
1:C:25:LYS:HZ2	1:C:78:GLN:NE2	2.14	0.46
1:C:25:LYS:HZ2	1:C:78:GLN:HE22	1.61	0.45
1:D:253:MET:CE	1:D:353:MET:HE1	2.46	0.45
1:E:7:GLU:OE1	1:E:7:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ALA:O	1:E:203:VAL:HG23	2.15	0.45
1:A:100:ASN:ND2	1:A:156:ARG:HH12	2.15	0.45
1:C:180:TYR:CG	1:C:181:PRO:HA	2.51	0.45
1:B:313:ILE:HD13	1:B:313:ILE:HA	1.73	0.45
1:B:357:TYR:O	1:B:359:ASN:N	2.49	0.45
1:C:14:THR:OG1	1:C:15:SER:N	2.49	0.45
1:C:174:TYR:CD2	1:C:192:VAL:HG21	2.52	0.45
1:E:61:ASP:OD2	1:E:444:ARG:NH1	2.50	0.45
1:E:298:PHE:CZ	1:E:345:ALA:HB3	2.51	0.45
1:A:254:GLU:HG3	1:A:262:PRO:HG3	1.99	0.45
1:A:416:TRP:CD1	1:A:417:THR:HB	2.52	0.45
1:A:426:ASN:O	1:A:427:ALA:C	2.60	0.45
1:F:389:ARG:O	1:F:393:LEU:HG	2.17	0.45
1:A:9:TRP:N	1:A:9:TRP:CD1	2.84	0.45
1:C:359:ASN:ND2	1:C:409:ASN:H	2.13	0.45
1:E:254:GLU:HB2	1:E:262:PRO:HD3	1.97	0.45
1:E:317:TRP:HA	1:E:321:TRP:CZ2	2.51	0.45
1:C:16:GLY:N	1:C:17:PRO:CD	2.80	0.45
1:D:331:ARG:NH2	1:D:333:MET:SD	2.90	0.45
1:F:80:THR:CG2	1:F:123:PRO:HG3	2.46	0.45
1:F:140:ASP:O	1:F:143:VAL:HB	2.17	0.45
1:A:16:GLY:N	1:A:17:PRO:CD	2.80	0.45
1:A:100:ASN:HD21	1:A:156:ARG:HH22	1.64	0.45
1:E:122:LEU:HD13	1:E:133:TRP:CE2	2.51	0.45
1:F:317:TRP:CD1	1:F:321:TRP:CZ3	3.04	0.45
1:A:100:ASN:HD22	1:A:156:ARG:HH12	1.65	0.44
1:A:359:ASN:HD21	1:A:409:ASN:H	1.65	0.44
1:F:277:GLN:NE2	1:F:277:GLN:CA	2.77	0.44
1:B:381:THR:O	1:B:381:THR:OG1	2.35	0.44
1:C:25:LYS:NZ	1:C:78:GLN:NE2	2.64	0.44
1:F:159:ASP:HA	1:F:293:TYR:OH	2.17	0.44
1:E:448:ALA:O	1:E:449:SER:C	2.60	0.44
1:F:144:ALA:O	1:F:147:LYS:HB2	2.18	0.44
1:B:139:VAL:O	1:B:143:VAL:HG23	2.18	0.44
1:B:371:ILE:HG13	1:B:388:TYR:CE1	2.52	0.44
1:F:313:ILE:HD13	1:F:313:ILE:HA	1.58	0.44
1:C:178:PHE:O	1:C:179:HIS:HD2	2.00	0.44
1:E:404:ILE:O	1:E:407:GLY:N	2.44	0.44
1:E:99:TYR:O	1:E:102:VAL:HB	2.17	0.44
1:A:14:THR:OG1	1:A:15:SER:N	2.47	0.44
1:A:279:THR:HG23	1:A:281:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:SER:O	1:C:444:ARG:NH2	2.42	0.44
1:D:249:ASN:N	1:D:249:ASN:HD22	2.14	0.44
1:D:426:ASN:O	1:D:427:ALA:C	2.60	0.44
1:D:445:ARG:HG3	1:D:445:ARG:HH11	1.81	0.44
1:A:445:ARG:HA	1:A:446:PRO:HD3	1.67	0.44
1:F:23:PHE:C	1:F:25:LYS:H	2.25	0.44
1:F:334:ASN:HB2	1:F:341:ILE:HD11	1.98	0.44
1:F:438:ASN:C	1:F:438:ASN:OD1	2.61	0.44
1:D:122:LEU:HD21	1:D:132:GLY:CA	2.48	0.43
1:B:312:VAL:HG23	1:B:313:ILE:N	2.33	0.43
1:B:314:SER:HA	1:B:315:PRO:HD2	1.91	0.43
1:C:8:PHE:CE1	1:C:412:GLY:N	2.86	0.43
1:D:61:ASP:O	1:D:65:LEU:HG	2.18	0.43
1:E:276:TRP:CD1	1:E:276:TRP:C	2.96	0.43
1:F:160:TRP:CB	1:F:219:ILE:CG2	2.91	0.43
1:C:313:ILE:HD13	1:C:313:ILE:HA	1.67	0.43
1:D:12:GLY:HA3	1:D:418:PRO:HG3	1.99	0.43
1:E:74:ARG:HB2	1:E:114:VAL:HB	1.99	0.43
1:F:194:TYR:O	1:F:197:ALA:HB3	2.19	0.43
1:A:180:TYR:CG	1:A:181:PRO:HA	2.53	0.43
1:B:375:ASP:O	1:B:378:ARG:HG2	2.19	0.43
1:C:216:ASP:OD1	1:C:216:ASP:N	2.52	0.43
1:E:44:ASP:O	1:E:45:TYR:HB2	2.18	0.43
1:F:190:VAL:HG21	1:F:274:VAL:HG13	2.00	0.43
1:A:313:ILE:HD12	1:A:313:ILE:HA	1.84	0.43
1:C:9:TRP:CD1	1:C:9:TRP:N	2.85	0.43
1:E:312:VAL:HG23	1:E:313:ILE:N	2.33	0.43
1:E:344:GLU:HG3	1:E:399:TYR:CE1	2.54	0.43
1:F:297:ASN:HD22	1:F:366:GLU:HB2	1.78	0.43
1:B:445:ARG:HH11	1:B:445:ARG:HG2	1.81	0.43
1:C:426:ASN:O	1:C:427:ALA:C	2.59	0.43
1:E:334:ASN:OD1	1:E:334:ASN:C	2.61	0.43
1:F:122:LEU:HD21	1:F:132:GLY:HA3	2.00	0.43
1:F:328:MET:O	1:F:331:ARG:HD3	2.19	0.43
1:E:58:ILE:HG12	1:E:102:VAL:HG22	2.00	0.43
1:F:135:SER:OG	1:F:138:VAL:HG23	2.18	0.43
1:C:15:SER:OG	1:C:18:GLN:NE2	2.43	0.42
1:E:162:VAL:HG11	1:E:200:THR:HA	2.00	0.42
1:B:74:ARG:HB2	1:B:114:VAL:HB	2.01	0.42
1:D:122:LEU:HD13	1:D:133:TRP:CE2	2.54	0.42
1:C:262:PRO:O	1:C:266:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:PRO:HD2	1:D:340:GLU:O	2.20	0.42
1:D:313:ILE:HD13	1:D:313:ILE:HA	1.66	0.42
1:E:7:GLU:OE1	1:E:7:GLU:CA	2.68	0.42
1:F:74:ARG:C	1:F:74:ARG:HD2	2.43	0.42
1:B:242:HIS:CE1	2:B:2003:HOH:O	2.53	0.42
1:C:53:ASP:OD1	1:C:56:HIS:CD2	2.63	0.42
1:F:11:GLY:C	1:F:414:HIS:HD2	2.27	0.42
1:F:222:ILE:HG23	1:F:365:SER:OG	2.18	0.42
1:A:246:LEU:HA	1:A:250:ASP:HB2	2.00	0.42
1:E:127:TYR:HA	1:E:132:GLY:H	1.84	0.42
1:B:6:LYS:C	1:B:7:GLU:HG2	2.45	0.42
1:F:204:ILE:HD12	1:F:219:ILE:HD13	2.00	0.42
1:B:12:GLY:HA3	1:B:418:PRO:HG3	2.02	0.42
1:D:371:ILE:HG22	1:D:372:SER:N	2.34	0.42
1:B:270:LYS:O	1:B:271:LYS:C	2.62	0.42
1:E:122:LEU:HD21	1:E:132:GLY:CA	2.49	0.42
1:F:86:PHE:O	1:F:141:LEU:HD22	2.19	0.42
1:F:318:SER:O	1:F:319:PRO:C	2.63	0.42
1:B:27:HIS:HB2	1:B:80:THR:HB	2.02	0.42
1:B:68:LEU:O	1:B:454:LYS:HB2	2.18	0.42
1:E:116:ASN:ND2	1:E:164:ASN:HB2	2.35	0.42
1:F:161:PHE:HA	1:F:220:GLY:O	2.20	0.42
1:F:243:PHE:O	1:F:246:LEU:N	2.53	0.42
1:A:301:PRO:HG3	1:A:342:TYR:HB3	2.01	0.42
1:B:190:VAL:HG21	1:B:274:VAL:HG13	2.02	0.42
1:E:363:PHE:CZ	1:E:365:SER:HB3	2.54	0.42
1:F:223:LEU:HB3	1:F:224:ASN:H	1.70	0.42
1:C:314:SER:HA	1:C:315:PRO:HD2	1.74	0.41
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.92	0.41
1:B:279:THR:HG21	1:B:281:GLU:HB2	2.01	0.41
1:B:417:THR:O	1:B:433:GLY:HA2	2.19	0.41
1:B:461:ARG:HE	1:B:461:ARG:HB2	1.57	0.41
1:D:253:MET:HE1	1:D:353:MET:HE1	2.01	0.41
1:B:353:MET:HE2	1:B:357:TYR:CD2	2.56	0.41
1:D:52:SER:O	1:D:444:ARG:NH2	2.48	0.41
1:D:248:ASN:C	1:D:249:ASN:HD22	2.28	0.41
1:E:447:LYS:O	1:E:450:ALA:HB3	2.21	0.41
1:F:328:MET:O	1:F:331:ARG:CD	2.68	0.41
1:F:332:ARG:O	1:F:340:GLU:HA	2.20	0.41
1:B:180:TYR:CG	1:B:181:PRO:HA	2.56	0.41
1:D:294:LEU:O	1:D:362:TRP:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ARG:HE	1:D:376:ARG:HB2	1.51	0.41
1:D:281:GLU:CD	1:D:281:GLU:H	2.28	0.41
1:E:313:ILE:HD13	1:E:313:ILE:HA	1.90	0.41
1:F:117:LEU:HB2	1:F:162:VAL:O	2.21	0.41
1:F:180:TYR:CG	1:F:181:PRO:HA	2.56	0.41
1:A:81:ARG:HD2	1:A:99:TYR:CE2	2.55	0.41
1:B:357:TYR:C	1:B:359:ASN:N	2.74	0.41
1:C:116:ASN:ND2	1:C:164:ASN:HB2	2.34	0.41
1:C:219:ILE:HG12	1:C:220:GLY:N	2.36	0.41
1:D:250:ASP:O	1:D:251:LEU:C	2.64	0.41
1:F:74:ARG:HB2	1:F:114:VAL:HB	2.02	0.41
1:B:22:ARG:O	1:B:23:PHE:C	2.63	0.41
1:B:106:CYS:HB3	1:B:111:ILE:O	2.21	0.41
1:D:22:ARG:O	1:D:23:PHE:C	2.61	0.41
1:E:73:TYR:CE1	1:E:75:THR:HB	2.56	0.41
1:A:247:TRP:NE1	1:A:319:PRO:HG3	2.36	0.41
1:A:318:SER:O	1:A:319:PRO:C	2.63	0.41
1:A:400:LEU:HD11	1:A:410:CYS:SG	2.61	0.41
1:D:261:PHE:HA	1:D:262:PRO:HD3	1.95	0.41
1:F:350:ALA:O	1:F:353:MET:HB2	2.20	0.41
1:A:225:LEU:HD13	1:A:253:MET:HG3	2.03	0.41
1:B:22:ARG:HD3	1:B:49:ASP:OD1	2.21	0.41
1:C:225:LEU:HD21	1:C:353:MET:CE	2.49	0.41
1:D:27:HIS:HB2	1:D:80:THR:HB	2.02	0.41
1:D:122:LEU:HD21	1:D:132:GLY:HA2	2.01	0.41
1:E:251:LEU:C	1:E:251:LEU:CD2	2.91	0.41
1:F:138:VAL:O	1:F:139:VAL:C	2.62	0.41
1:A:248:ASN:C	1:A:249:ASN:HD22	2.29	0.41
1:B:42:PHE:O	1:B:43:TYR:C	2.62	0.41
1:C:72:SER:HA	1:C:111:ILE:HG23	2.03	0.41
1:C:419:ILE:O	1:C:420:ASP:C	2.63	0.41
1:E:161:PHE:HA	1:E:220:GLY:O	2.21	0.41
1:C:29:ASN:HD22	1:C:78:GLN:NE2	2.18	0.40
1:C:441:THR:O	1:C:442:GLN:HB2	2.20	0.40
1:E:362:TRP:CZ2	1:E:410:CYS:HB2	2.56	0.40
1:F:297:ASN:ND2	1:F:366:GLU:CB	2.77	0.40
1:F:397:LEU:HD13	1:F:397:LEU:HA	1.98	0.40
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.98	0.40
1:F:366:GLU:HG2	1:F:416:TRP:CE3	2.57	0.40
1:D:204:ILE:HG12	1:D:219:ILE:HD13	2.02	0.40
1:F:78:GLN:HG3	1:F:121:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ASP:OD2	1:F:188:LYS:HG3	2.21	0.40
1:F:199:ALA:O	1:F:203:VAL:CG2	2.54	0.40
1:F:200:THR:O	1:F:204:ILE:HG12	2.22	0.40
1:C:15:SER:HB3	1:C:119:HIS:CD2	2.57	0.40
1:C:364:LEU:HD23	1:C:413:TYR:CD1	2.56	0.40
1:E:180:TYR:CD1	1:E:181:PRO:HA	2.56	0.40
1:E:310:ILE:HA	1:E:311:PRO:HD3	1.87	0.40
1:F:165:GLU:HA	1:F:166:PRO:HD2	1.92	0.40
1:F:279:THR:HA	1:F:280:PRO:HD3	1.86	0.40
1:A:116:ASN:HA	1:A:161:PHE:O	2.21	0.40
1:A:124:ILE:O	1:A:124:ILE:HG13	2.22	0.40
1:C:331:ARG:NH1	1:C:333:MET:HB2	2.36	0.40
1:D:397:LEU:O	1:D:398:THR:C	2.64	0.40
1:E:397:LEU:HB3	1:E:462:LEU:HD11	2.02	0.40
1:E:436:GLU:O	1:E:444:ARG:HA	2.21	0.40
1:F:297:ASN:ND2	1:F:366:GLU:N	2.69	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	459/479 (96%)	438 (95%)	20 (4%)	1 (0%)	43	63
1	B	459/479 (96%)	429 (94%)	26 (6%)	4 (1%)	14	27
1	C	459/479 (96%)	425 (93%)	32 (7%)	2 (0%)	30	49
1	D	459/479 (96%)	424 (92%)	34 (7%)	1 (0%)	43	63
1	E	459/479 (96%)	425 (93%)	30 (6%)	4 (1%)	14	27
1	F	459/479 (96%)	409 (89%)	46 (10%)	4 (1%)	14	27
All	All	2754/2874 (96%)	2550 (93%)	188 (7%)	16 (1%)	21	38

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	359	ASN
1	B	375	ASP
1	D	336	ASP
1	E	274	VAL
1	E	359	ASN
1	F	24	ALA
1	B	274	VAL
1	E	51	ALA
1	F	375	ASP
1	B	358	ASP
1	F	73	TYR
1	A	212	ALA
1	E	262	PRO
1	C	154	GLY
1	B	210	GLY
1	F	113	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	389/404 (96%)	371 (95%)	18 (5%)	24	48
1	B	389/404 (96%)	367 (94%)	22 (6%)	18	39
1	C	389/404 (96%)	364 (94%)	25 (6%)	16	33
1	D	389/404 (96%)	365 (94%)	24 (6%)	16	34
1	E	389/404 (96%)	368 (95%)	21 (5%)	20	41
1	F	389/404 (96%)	345 (89%)	44 (11%)	5	12
All	All	2334/2424 (96%)	2180 (93%)	154 (7%)	15	32

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU

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Mol	Chain	Res	Type
1	A	83	ILE
1	A	187	LYS
1	A	218	ARG
1	A	226	THR
1	A	234	SER
1	A	251	LEU
1	A	274	VAL
1	A	277	GLN
1	A	279	THR
1	A	293	TYR
1	A	313	ILE
1	A	327	LEU
1	A	331	ARG
1	A	333	MET
1	A	444	ARG
1	A	445	ARG
1	A	461	ARG
1	B	2	LEU
1	B	60	SER
1	B	135	SER
1	B	218	ARG
1	B	226	THR
1	B	233	GLN
1	B	274	VAL
1	B	277	GLN
1	B	279	THR
1	B	293	TYR
1	B	313	ILE
1	B	327	LEU
1	B	328	MET
1	B	331	ARG
1	B	333	MET
1	B	337	LYS
1	B	359	ASN
1	B	378	ARG
1	B	380	GLU
1	B	397	LEU
1	B	444	ARG
1	B	445	ARG
1	C	2	LEU
1	C	103	ILE
1	C	218	ARG

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Mol	Chain	Res	Type
1	C	226	THR
1	C	260	LYS
1	C	274	VAL
1	C	277	GLN
1	C	279	THR
1	C	286	ILE
1	C	288	GLU
1	C	293	TYR
1	C	313	ILE
1	C	314	SER
1	C	327	LEU
1	C	331	ARG
1	C	333	MET
1	C	337	LYS
1	C	359	ASN
1	C	365	SER
1	C	397	LEU
1	C	402	LYS
1	C	444	ARG
1	C	446	PRO
1	C	455	LYS
1	C	462	LEU
1	D	2	LEU
1	D	50	THR
1	D	183	ILE
1	D	218	ARG
1	D	219	ILE
1	D	226	THR
1	D	234	SER
1	D	260	LYS
1	D	263	GLU
1	D	274	VAL
1	D	277	GLN
1	D	279	THR
1	D	293	TYR
1	D	313	ILE
1	D	314	SER
1	D	316	SER
1	D	331	ARG
1	D	337	LYS
1	D	378	ARG
1	D	397	LEU

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Mol	Chain	Res	Type
1	D	405	GLU
1	D	444	ARG
1	D	455	LYS
1	D	461	ARG
1	E	2	LEU
1	E	7	GLU
1	E	14	THR
1	E	40	ASP
1	E	200	THR
1	E	218	ARG
1	E	226	THR
1	E	238	MET
1	E	277	GLN
1	E	278	SER
1	E	293	TYR
1	E	314	SER
1	E	331	ARG
1	E	333	MET
1	E	359	ASN
1	E	365	SER
1	E	381	THR
1	E	397	LEU
1	E	405	GLU
1	E	408	SER
1	E	444	ARG
1	F	2	LEU
1	F	58	ILE
1	F	67	SER
1	F	81	ARG
1	F	103	ILE
1	F	120	PHE
1	F	135	SER
1	F	162	VAL
1	F	183	ILE
1	F	184	VAL
1	F	185	ASP
1	F	187	LYS
1	F	209	ARG
1	F	219	ILE
1	F	221	THR
1	F	226	THR
1	F	233	GLN

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Mol	Chain	Res	Type
1	F	234	SER
1	F	254	GLU
1	F	274	VAL
1	F	277	GLN
1	F	281	GLU
1	F	285	LEU
1	F	293	TYR
1	F	308	ASP
1	F	312	VAL
1	F	313	ILE
1	F	314	SER
1	F	327	LEU
1	F	331	ARG
1	F	353	MET
1	F	358	ASP
1	F	359	ASN
1	F	360	ILE
1	F	365	SER
1	F	375	ASP
1	F	380	GLU
1	F	381	THR
1	F	390	ILE
1	F	397	LEU
1	F	405	GLU
1	F	410	CYS
1	F	444	ARG
1	F	461	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	57	GLN
1	A	78	GLN
1	A	100	ASN
1	A	116	ASN
1	A	249	ASN
1	A	289	ASN
1	A	297	ASN
1	A	359	ASN
1	A	383	GLN
1	A	430	ASN

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Mol	Chain	Res	Type
1	B	27	HIS
1	B	56	HIS
1	B	100	ASN
1	B	116	ASN
1	B	249	ASN
1	B	297	ASN
1	B	359	ASN
1	B	385	GLN
1	B	459	HIS
1	C	18	GLN
1	C	56	HIS
1	C	78	GLN
1	C	100	ASN
1	C	116	ASN
1	C	119	HIS
1	C	152	GLN
1	C	177	GLN
1	C	179	HIS
1	C	205	GLN
1	C	248	ASN
1	C	249	ASN
1	C	297	ASN
1	C	359	ASN
1	C	383	GLN
1	D	56	HIS
1	D	57	GLN
1	D	78	GLN
1	D	100	ASN
1	D	249	ASN
1	D	258	HIS
1	D	297	ASN
1	D	359	ASN
1	D	385	GLN
1	D	459	HIS
1	E	56	HIS
1	E	70	HIS
1	E	100	ASN
1	E	152	GLN
1	E	195	ASN
1	E	249	ASN
1	E	289	ASN
1	E	297	ASN

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Mol	Chain	Res	Type
1	E	359	ASN
1	E	367	ASN
1	E	385	GLN
1	E	426	ASN
1	F	56	HIS
1	F	78	GLN
1	F	88	GLN
1	F	100	ASN
1	F	119	HIS
1	F	137	HIS
1	F	152	GLN
1	F	164	ASN
1	F	249	ASN
1	F	277	GLN
1	F	289	ASN
1	F	297	ASN
1	F	359	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	461/479 (96%)	-0.46	2 (0%) 88 86	24, 40, 63, 93	1 (0%)
1	B	461/479 (96%)	-0.37	3 (0%) 84 81	25, 41, 63, 84	1 (0%)
1	C	461/479 (96%)	-0.27	3 (0%) 84 81	26, 44, 67, 91	1 (0%)
1	D	461/479 (96%)	-0.31	2 (0%) 88 86	25, 42, 64, 82	1 (0%)
1	E	461/479 (96%)	-0.08	4 (0%) 81 78	28, 48, 70, 102	2 (0%)
1	F	461/479 (96%)	0.44	23 (4%) 34 30	27, 53, 75, 97	2 (0%)
All	All	2766/2874 (96%)	-0.17	37 (1%) 75 71	24, 45, 69, 102	8 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	380	GLU	4.9
1	E	6	LYS	4.7
1	F	6	LYS	4.4
1	A	6	LYS	3.9
1	E	315	PRO	3.9
1	B	312	VAL	3.6
1	C	6	LYS	3.6
1	E	380	GLU	3.5
1	B	313	ILE	3.4
1	A	313	ILE	2.9
1	F	280	PRO	2.9
1	D	312	VAL	2.7
1	F	279	THR	2.7
1	F	157	VAL	2.7
1	F	153	PHE	2.6
1	C	312	VAL	2.6
1	B	6	LYS	2.6
1	D	313	ILE	2.6
1	F	283	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	261	PHE	2.5
1	F	257	VAL	2.4
1	F	200	THR	2.4
1	F	11	GLY	2.4
1	F	194	TYR	2.4
1	F	278	SER	2.4
1	E	313	ILE	2.3
1	F	350	ALA	2.2
1	C	315	PRO	2.2
1	F	68	LEU	2.2
1	F	107	LEU	2.1
1	F	221	THR	2.1
1	F	201	ALA	2.1
1	F	196	LEU	2.1
1	F	285	LEU	2.0
1	F	462	LEU	2.0
1	F	270	LYS	2.0
1	F	315	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.