



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:39 PM UTC

PDB ID : 2R6D / pdb_00002r6d
Title : Crystal Form B1
Authors : Bailey, S.; Eliason, W.K.; Steitz, T.A.
Deposited on : 2007-09-05
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

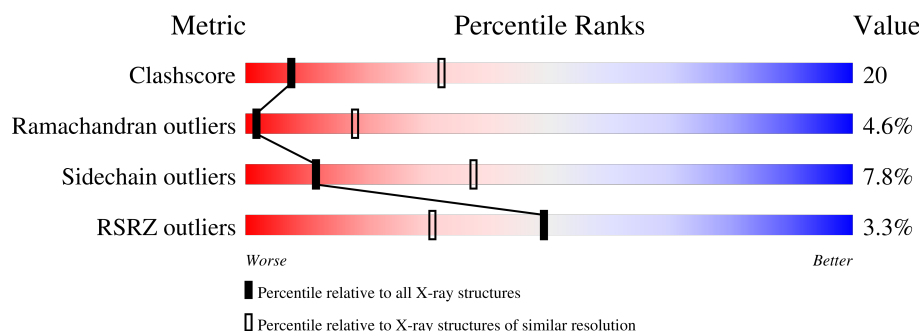
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	454	4% 52% 30% 5% • 11%
1	B	454	2% 53% 23% 6% • 17%
1	C	454	3% 56% 25% 5% • 12%
1	D	454	4% 52% 24% 5% • 17%
1	E	454	3% 58% 22% 6% • 14%
1	F	454	2% 57% 23% 5% • 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18085 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.

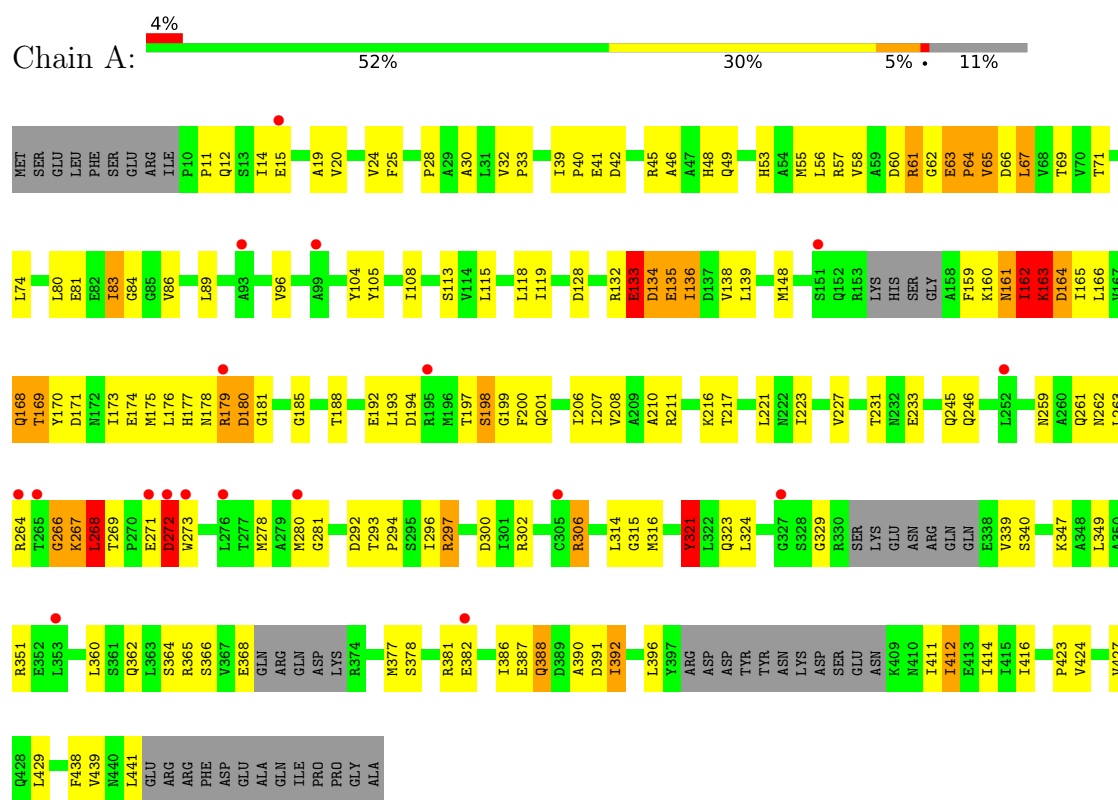
- Molecule 1 is a protein called Replicative helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3138	1969	544	611	14			
1	B	376	Total	C	N	O	S	0	0	0
			2897	1820	500	564	13			
1	C	399	Total	C	N	O	S	0	0	0
			3089	1938	534	603	14			
1	D	376	Total	C	N	O	S	0	0	0
			2897	1820	500	564	13			
1	E	392	Total	C	N	O	S	0	0	0
			3032	1905	521	593	13			
1	F	392	Total	C	N	O	S	0	0	0
			3032	1905	521	593	13			

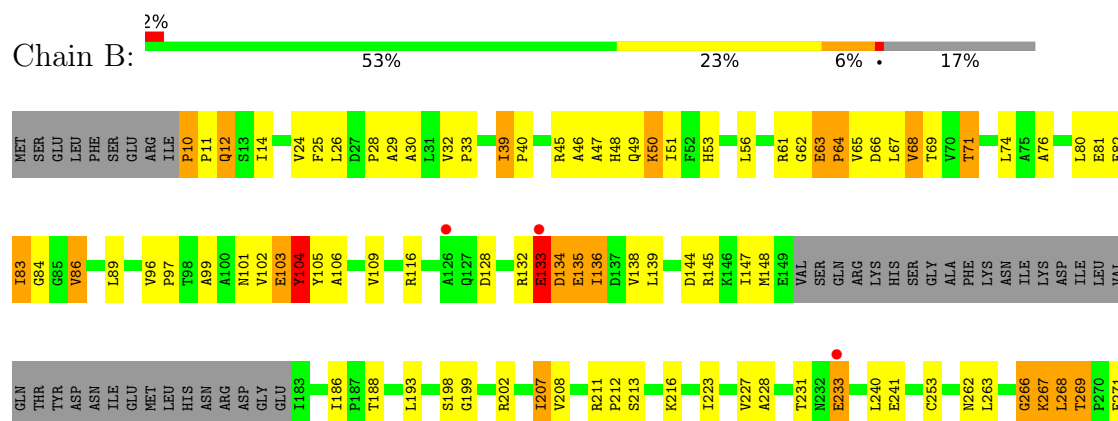
3 Residue-property plots

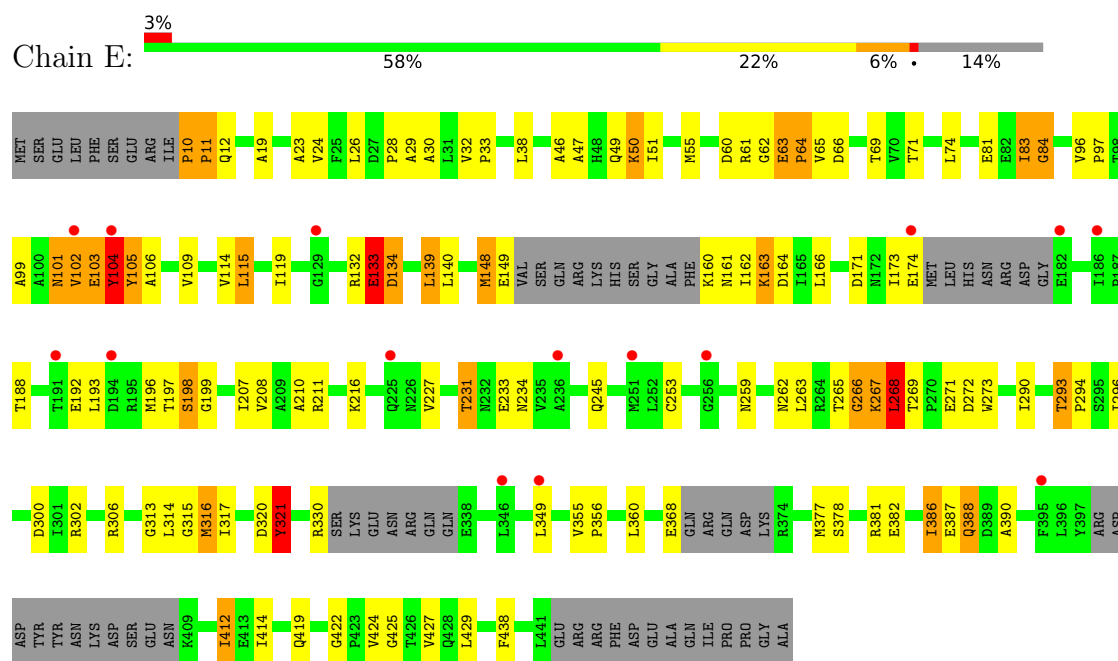
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Replicative helicase

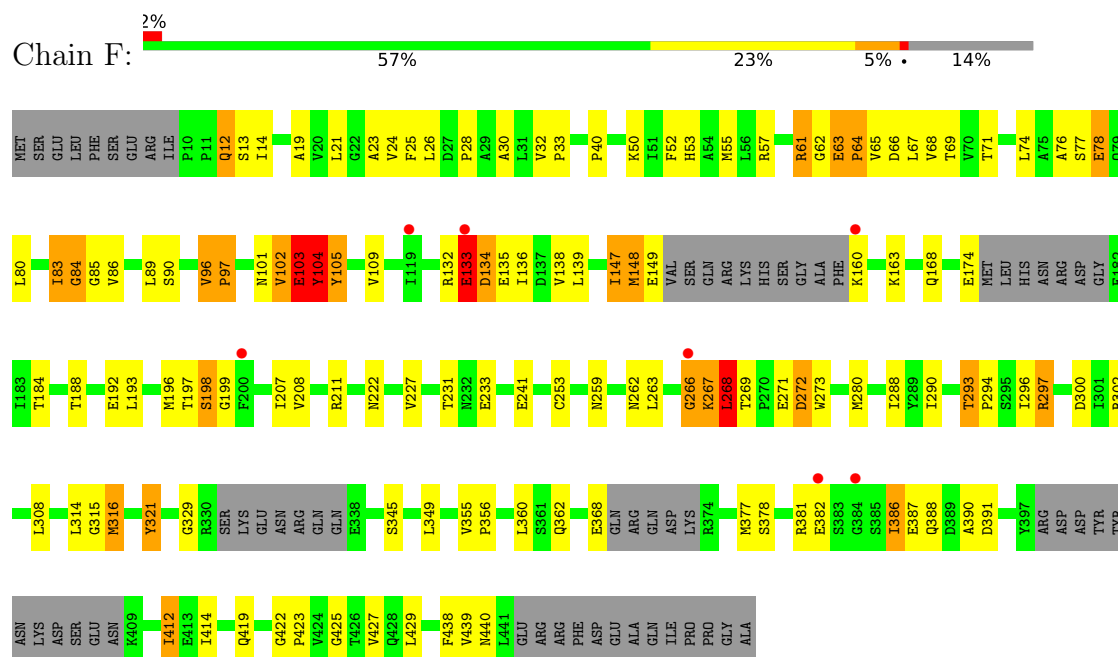


• Molecule 1: Replicative helicase





• Molecule 1: Replicative helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	371.26Å 110.30Å 112.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-3.70) 97.3 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.71Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.309 , 0.322 0.289 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	145.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 199.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.077 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18085	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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	0.57	0/3173	0.98	10/4285 (0.2%)
1	B	0.58	0/2929	1.04	19/3957 (0.5%)
1	C	0.58	3/3123 (0.1%)	1.05	14/4218 (0.3%)
1	D	0.52	0/2929	1.02	16/3957 (0.4%)
1	E	0.50	0/3064	1.00	15/4138 (0.4%)
1	F	0.54	0/3064	1.03	19/4138 (0.5%)
All	All	0.55	3/18282 (0.0%)	1.02	93/24693 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	2
1	D	1	1
1	E	1	0
1	F	1	1
All	All	5	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	GLU	C-N	7.41	1.44	1.33
1	C	32	VAL	CA-CB	6.02	1.57	1.54
1	C	61	ARG	CA-C	5.65	1.55	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	GLU	N-CA-C	11.37	125.42	112.57
1	E	10	PRO	CA-C-N	9.76	132.04	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	PRO	C-N-CA	9.76	132.04	119.84
1	C	293	THR	CA-C-N	9.60	131.83	119.84
1	C	293	THR	C-N-CA	9.60	131.83	119.84
1	C	174	GLU	O-C-N	9.35	132.12	122.03
1	A	321	TYR	N-CA-C	7.51	126.79	110.80
1	B	321	TYR	N-CA-C	7.43	126.63	110.80
1	E	103	GLU	N-CA-C	7.40	121.21	112.93
1	C	321	TYR	N-CA-C	7.30	126.34	110.80
1	C	174	GLU	N-CA-C	-7.20	103.04	111.03
1	D	84	GLY	N-CA-C	-7.14	102.56	112.13
1	F	321	TYR	N-CA-C	7.07	125.85	110.80
1	D	103	GLU	CA-C-N	7.00	134.30	121.70
1	D	103	GLU	C-N-CA	7.00	134.30	121.70
1	D	133	GLU	CA-C-N	6.97	134.25	121.70
1	D	133	GLU	C-N-CA	6.97	134.25	121.70
1	E	422	GLY	CA-C-N	6.92	126.85	120.21
1	E	422	GLY	C-N-CA	6.92	126.85	120.21
1	E	103	GLU	CA-C-N	6.90	134.12	121.70
1	E	103	GLU	C-N-CA	6.90	134.12	121.70
1	E	84	GLY	N-CA-C	-6.84	102.81	112.60
1	A	65	VAL	N-CA-C	6.81	117.69	107.75
1	B	103	GLU	CA-C-N	6.74	133.84	121.70
1	B	103	GLU	C-N-CA	6.74	133.84	121.70
1	D	321	TYR	N-CA-C	6.67	125.00	110.80
1	C	133	GLU	CA-C-N	6.62	133.62	121.70
1	C	133	GLU	C-N-CA	6.62	133.62	121.70
1	F	103	GLU	CA-C-N	6.58	133.55	121.70
1	F	103	GLU	C-N-CA	6.58	133.55	121.70
1	F	133	GLU	CA-C-N	6.57	133.53	121.70
1	F	133	GLU	C-N-CA	6.57	133.53	121.70
1	F	103	GLU	N-CA-C	6.54	118.51	109.54
1	C	84	GLY	N-CA-C	-6.44	97.91	113.18
1	C	104	TYR	N-CA-C	6.42	124.48	110.80
1	E	293	THR	CA-C-N	6.35	127.78	119.84
1	E	293	THR	C-N-CA	6.35	127.78	119.84
1	B	26	LEU	N-CA-C	6.16	117.87	111.03
1	B	293	THR	CA-C-N	6.15	127.53	119.84
1	B	293	THR	C-N-CA	6.15	127.53	119.84
1	E	133	GLU	CA-C-N	6.14	132.75	121.70
1	E	133	GLU	C-N-CA	6.14	132.75	121.70
1	F	133	GLU	N-CA-C	6.08	123.75	110.80
1	E	321	TYR	N-CA-C	6.05	123.69	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	GLU	N-CA-C	6.04	123.66	110.80
1	A	133	GLU	CA-C-N	5.86	132.25	121.70
1	A	133	GLU	C-N-CA	5.86	132.25	121.70
1	F	293	THR	CA-C-N	5.84	127.14	119.84
1	F	293	THR	C-N-CA	5.84	127.14	119.84
1	B	133	GLU	CA-C-N	5.81	132.16	121.70
1	B	133	GLU	C-N-CA	5.81	132.16	121.70
1	D	103	GLU	N-CA-C	5.80	117.41	110.44
1	C	133	GLU	N-CA-C	5.73	123.01	110.80
1	F	321	TYR	CA-C-N	5.70	127.92	120.28
1	F	321	TYR	C-N-CA	5.70	127.92	120.28
1	D	39	ILE	CA-C-N	5.69	126.96	119.84
1	D	39	ILE	C-N-CA	5.69	126.96	119.84
1	D	104	TYR	CA-C-N	5.67	131.91	121.70
1	D	104	TYR	C-N-CA	5.67	131.91	121.70
1	B	86	VAL	N-CA-C	-5.62	104.69	112.50
1	A	293	THR	CA-C-N	5.62	126.86	119.84
1	A	293	THR	C-N-CA	5.62	126.86	119.84
1	F	422	GLY	CA-C-N	5.54	126.32	120.11
1	F	422	GLY	C-N-CA	5.54	126.32	120.11
1	B	39	ILE	CA-C-N	5.51	126.73	119.84
1	B	39	ILE	C-N-CA	5.51	126.73	119.84
1	F	26	LEU	N-CA-C	5.48	117.33	111.36
1	D	321	TYR	CA-C-N	5.48	127.62	120.28
1	D	321	TYR	C-N-CA	5.48	127.62	120.28
1	B	10	PRO	CA-C-N	5.46	125.73	119.83
1	B	10	PRO	C-N-CA	5.46	125.73	119.83
1	F	84	GLY	N-CA-C	-5.45	100.26	113.18
1	C	100	ALA	N-CA-C	-5.30	106.32	112.89
1	C	174	GLU	CA-C-O	-5.28	115.46	120.90
1	B	272	ASP	N-CA-C	-5.25	105.72	111.82
1	F	85	GLY	N-CA-C	-5.25	105.56	112.81
1	D	27	ASP	N-CA-C	5.23	121.36	109.81
1	B	133	GLU	N-CA-C	5.22	121.92	110.80
1	E	133	GLU	N-CA-C	5.21	121.89	110.80
1	A	272	ASP	N-CA-C	-5.19	105.80	111.82
1	F	105	TYR	N-CA-C	-5.17	99.79	110.80
1	B	29	ALA	N-CA-C	-5.15	107.02	113.15
1	B	104	TYR	CA-C-N	5.13	130.93	121.70
1	B	104	TYR	C-N-CA	5.13	130.93	121.70
1	D	96	VAL	CA-C-N	5.12	124.43	118.85
1	D	96	VAL	C-N-CA	5.12	124.43	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	TYR	N-CA-CB	5.11	119.12	110.49
1	E	104	TYR	CA-CB-CG	-5.07	104.78	113.90
1	A	321	TYR	CA-C-N	5.04	127.03	120.28
1	A	321	TYR	C-N-CA	5.04	127.03	120.28
1	B	84	GLY	N-CA-C	-5.02	101.28	113.18
1	F	104	TYR	CA-C-N	5.01	131.11	121.54
1	F	104	TYR	C-N-CA	5.01	131.11	121.54

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	104	TYR	CA
1	C	104	TYR	CA
1	D	104	TYR	CA
1	E	104	TYR	CA
1	F	104	TYR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	103	GLU	Peptide
1	C	174	GLU	Mainchain
1	D	104	TYR	Peptide
1	F	104	TYR	Peptide

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	3138	0	3190	148	0
1	B	2897	0	2953	135	0
1	C	3089	0	3141	152	2
1	D	2897	0	2953	162	0
1	E	3032	0	3087	117	0
1	F	3032	0	3087	114	2
All	All	18085	0	18411	742	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (742) 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:A:133:GLU:N	1:A:134:ASP:HB2	1.33	1.43
1:E:133:GLU:N	1:E:134:ASP:HB2	1.36	1.40
1:F:133:GLU:N	1:F:134:ASP:HB2	1.39	1.38
1:C:133:GLU:N	1:C:134:ASP:HB2	1.32	1.35
1:E:330:ARG:NH1	1:F:148:MET:O	1.63	1.32
1:C:133:GLU:H	1:C:134:ASP:CB	1.43	1.30
1:B:133:GLU:N	1:B:134:ASP:HB2	1.42	1.30
1:A:133:GLU:H	1:A:134:ASP:CB	1.45	1.27
1:D:133:GLU:N	1:D:134:ASP:HB2	1.47	1.26
1:E:133:GLU:H	1:E:134:ASP:CB	1.48	1.23
1:C:174:GLU:O	1:C:177:HIS:N	1.73	1.22
1:D:133:GLU:H	1:D:134:ASP:CB	1.51	1.22
1:C:294:PRO:HB2	1:D:381:ARG:NE	1.58	1.18
1:F:133:GLU:H	1:F:134:ASP:CB	1.57	1.17
1:B:133:GLU:H	1:B:134:ASP:CB	1.62	1.13
1:D:62:GLY:HA2	1:D:63:GLU:HB3	1.31	1.11
1:F:63:GLU:H	1:F:64:PRO:HA	1.14	1.10
1:D:63:GLU:H	1:D:64:PRO:HA	1.12	1.07
1:C:104:TYR:HB3	1:C:105:TYR:HB2	1.34	1.06
1:D:135:GLU:HG2	1:D:330:ARG:HH21	1.16	1.05
1:B:133:GLU:H	1:B:134:ASP:HB2	0.91	1.03
1:B:268:LEU:HB2	1:C:177:HIS:HE1	1.19	1.03
1:D:133:GLU:H	1:D:134:ASP:HB2	0.87	1.02
1:E:104:TYR:HA	1:E:105:TYR:HB2	1.38	1.01
1:E:61:ARG:HB2	1:E:62:GLY:HA3	1.39	1.01
1:A:294:PRO:HG3	1:B:348:ALA:HA	1.40	0.99
1:D:135:GLU:HG2	1:D:330:ARG:NH2	1.78	0.99
1:E:330:ARG:CZ	1:F:148:MET:O	2.10	0.99
1:F:61:ARG:HB2	1:F:62:GLY:HA3	1.44	0.98
1:E:19:ALA:HA	1:E:96:VAL:HG21	1.44	0.97
1:C:61:ARG:HB2	1:C:62:GLY:HA3	1.44	0.96
1:A:306:ARG:NH2	1:B:103:GLU:OE2	1.99	0.96
1:B:104:TYR:HB3	1:B:105:TYR:HB2	1.44	0.96
1:E:63:GLU:H	1:E:64:PRO:HA	1.27	0.96
1:F:207:ILE:HD12	1:F:390:ALA:HB2	1.48	0.94
1:D:61:ARG:HB2	1:D:62:GLY:HA3	1.50	0.94
1:A:61:ARG:CB	1:A:62:GLY:HA3	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ILE:HD12	1:E:390:ALA:HB2	1.50	0.92
1:C:294:PRO:HB2	1:D:381:ARG:CD	1.98	0.92
1:D:145:ARG:NH1	1:D:328:SER:H	1.66	0.92
1:D:145:ARG:HD3	1:D:328:SER:OG	1.70	0.91
1:C:171:ASP:O	1:C:175:MET:HG3	1.70	0.91
1:D:145:ARG:HG3	1:D:341:GLU:OE1	1.70	0.91
1:D:145:ARG:HH11	1:D:328:SER:H	0.93	0.91
1:C:61:ARG:CB	1:C:62:GLY:HA3	2.00	0.90
1:E:104:TYR:CA	1:E:105:TYR:HB2	2.03	0.89
1:A:207:ILE:HD12	1:A:390:ALA:HB2	1.51	0.88
1:B:268:LEU:HB2	1:C:177:HIS:CE1	2.09	0.87
1:C:174:GLU:CG	1:C:175:MET:N	2.35	0.87
1:E:330:ARG:HG3	1:F:149:GLU:HG2	1.53	0.87
1:D:104:TYR:HB3	1:D:105:TYR:HB2	1.57	0.86
1:E:265:THR:HG23	1:F:423:PRO:HB3	1.57	0.85
1:F:101:ASN:O	1:F:103:GLU:N	2.07	0.85
1:D:145:ARG:HH11	1:D:328:SER:N	1.73	0.85
1:F:61:ARG:CB	1:F:62:GLY:HA3	2.04	0.84
1:B:63:GLU:H	1:B:64:PRO:HA	1.42	0.84
1:F:32:VAL:HB	1:F:33:PRO:HD3	1.58	0.83
1:F:104:TYR:HB3	1:F:105:TYR:HB2	1.60	0.83
1:D:32:VAL:HB	1:D:33:PRO:HD3	1.60	0.83
1:E:61:ARG:CB	1:E:62:GLY:HA3	2.08	0.83
1:A:227:VAL:O	1:A:231:THR:HG22	1.79	0.83
1:C:294:PRO:HG2	1:D:381:ARG:CZ	2.09	0.83
1:C:174:GLU:OE2	1:C:178:ASN:HB3	1.79	0.83
1:E:104:TYR:HB3	1:E:105:TYR:HB2	1.61	0.82
1:F:67:LEU:O	1:F:71:THR:HG23	1.79	0.82
1:D:265:THR:HG23	1:E:424:VAL:H	1.44	0.81
1:C:207:ILE:HD13	1:C:386:ILE:HG22	1.62	0.81
1:D:135:GLU:CG	1:D:330:ARG:HH21	1.92	0.81
1:D:142:GLU:N	1:D:328:SER:HB2	1.95	0.81
1:F:302:ARG:HG2	1:F:349:LEU:HD13	1.63	0.81
1:A:198:SER:N	1:A:199:GLY:HA2	1.96	0.80
1:C:148:MET:HE3	1:C:148:MET:HA	1.63	0.80
1:D:63:GLU:N	1:D:64:PRO:HA	1.96	0.80
1:A:246:GLN:NE2	1:B:420:ARG:HB3	1.97	0.80
1:D:19:ALA:HA	1:D:96:VAL:HG21	1.62	0.80
1:A:294:PRO:HG3	1:B:348:ALA:CA	2.11	0.79
1:D:62:GLY:HA2	1:D:63:GLU:CB	1.99	0.79
1:D:145:ARG:NH1	1:D:328:SER:N	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:SER:N	1:F:199:GLY:HA2	1.97	0.79
1:C:172:ASN:HA	1:C:175:MET:HB2	1.64	0.79
1:F:63:GLU:N	1:F:64:PRO:HA	1.96	0.79
1:C:175:MET:O	1:C:179:ARG:HD2	1.83	0.79
1:D:101:ASN:O	1:D:103:GLU:N	2.15	0.79
1:E:198:SER:N	1:E:199:GLY:HA2	1.98	0.78
1:C:198:SER:N	1:C:199:GLY:HA2	1.98	0.78
1:A:188:THR:HG21	1:A:193:LEU:HD23	1.65	0.78
1:E:32:VAL:HB	1:E:33:PRO:HD3	1.65	0.78
1:E:104:TYR:CB	1:E:105:TYR:HB2	2.13	0.78
1:B:347:LYS:HE3	1:B:351:ARG:CZ	2.14	0.78
1:E:207:ILE:HD13	1:E:386:ILE:HG22	1.67	0.77
1:C:104:TYR:CB	1:C:105:TYR:HB2	2.13	0.76
1:B:61:ARG:HB2	1:B:62:GLY:HA3	1.67	0.76
1:B:268:LEU:HD12	1:C:177:HIS:CE1	2.20	0.76
1:B:267:LYS:O	1:C:177:HIS:CE1	2.40	0.75
1:A:161:ASN:HD21	1:A:163:LYS:HG2	1.52	0.75
1:D:63:GLU:H	1:D:64:PRO:CA	1.98	0.75
1:C:306:ARG:HD3	1:D:32:VAL:HG13	1.69	0.75
1:D:62:GLY:CA	1:D:63:GLU:HB3	2.15	0.75
1:A:61:ARG:HB3	1:A:62:GLY:HA3	1.67	0.75
1:C:28:PRO:C	1:C:30:ALA:H	1.95	0.75
1:C:294:PRO:CB	1:D:381:ARG:NE	2.46	0.74
1:A:161:ASN:ND2	1:A:163:LYS:HG2	2.02	0.74
1:B:207:ILE:HD12	1:B:390:ALA:HB2	1.68	0.74
1:A:63:GLU:H	1:A:64:PRO:HA	1.52	0.74
1:C:241:GLU:HG3	1:D:378:SER:HB3	1.68	0.74
1:B:198:SER:N	1:B:199:GLY:HA2	2.01	0.74
1:E:66:ASP:H	1:E:69:THR:HG22	1.52	0.74
1:A:381:ARG:HH22	1:A:388:GLN:HE22	1.36	0.74
1:B:61:ARG:CB	1:B:62:GLY:HA3	2.18	0.73
1:F:207:ILE:HD13	1:F:386:ILE:HG22	1.70	0.73
1:B:67:LEU:O	1:B:71:THR:HG23	1.88	0.73
1:D:198:SER:N	1:D:199:GLY:HA2	2.03	0.72
1:D:273:TRP:CH2	1:E:173:ILE:HG22	2.24	0.72
1:C:63:GLU:H	1:C:64:PRO:HA	1.55	0.72
1:F:297:ARG:NH2	1:F:329:GLY:O	2.20	0.72
1:C:207:ILE:HD12	1:C:390:ALA:HB2	1.71	0.71
1:D:145:ARG:CG	1:D:341:GLU:OE1	2.39	0.71
1:A:245:GLN:HE22	1:B:202:ARG:HH12	1.39	0.70
1:F:269:THR:HB	1:F:272:ASP:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:MET:O	1:C:179:ARG:CD	2.39	0.70
1:D:66:ASP:H	1:D:69:THR:HG22	1.55	0.69
1:D:40:PRO:O	1:D:49:GLN:HG2	1.92	0.69
1:C:40:PRO:O	1:C:49:GLN:HG3	1.92	0.69
1:D:32:VAL:HG12	1:D:36:GLU:OE1	1.93	0.69
1:F:64:PRO:O	1:F:69:THR:HG21	1.92	0.69
1:A:159:PHE:HD1	1:A:160:LYS:H	1.40	0.69
1:D:136:ILE:HD12	1:E:115:LEU:HG	1.74	0.69
1:E:63:GLU:N	1:E:64:PRO:HA	2.06	0.69
1:C:241:GLU:O	1:D:377:MET:HB2	1.93	0.68
1:B:207:ILE:HD13	1:B:386:ILE:HG22	1.74	0.68
1:D:66:ASP:H	1:D:69:THR:CG2	2.07	0.68
1:D:61:ARG:CB	1:D:62:GLY:HA3	2.15	0.68
1:C:294:PRO:HG2	1:D:381:ARG:NH2	2.09	0.68
1:A:61:ARG:HB2	1:A:62:GLY:HA3	1.72	0.68
1:C:148:MET:HA	1:C:148:MET:CE	2.22	0.68
1:A:269:THR:HB	1:A:272:ASP:HB2	1.76	0.67
1:D:67:LEU:O	1:D:71:THR:HG23	1.94	0.67
1:E:330:ARG:NH2	1:F:149:GLU:HA	2.09	0.67
1:C:307:ARG:HE	1:D:36:GLU:CD	2.02	0.67
1:A:197:THR:O	1:A:198:SER:HB2	1.94	0.67
1:C:306:ARG:HD3	1:D:32:VAL:CG1	2.25	0.67
1:D:290:ILE:O	1:E:160:LYS:HB3	1.94	0.67
1:C:19:ALA:HA	1:C:96:VAL:HG21	1.74	0.67
1:C:307:ARG:NH2	1:D:36:GLU:OE2	2.27	0.67
1:C:175:MET:HB3	1:C:423:PRO:HB3	1.77	0.67
1:D:227:VAL:O	1:D:231:THR:HG22	1.95	0.66
1:C:320:ASP:HA	1:C:360:LEU:HD12	1.76	0.66
1:C:227:VAL:O	1:C:231:THR:HG22	1.95	0.66
1:A:294:PRO:HA	1:B:351:ARG:NH1	2.10	0.66
1:A:65:VAL:HA	1:A:69:THR:HG21	1.78	0.66
1:D:302:ARG:HG2	1:D:349:LEU:HD13	1.78	0.66
1:D:141:ASP:C	1:D:143:ALA:H	2.04	0.65
1:F:412:ILE:HG21	1:F:438:PHE:HE2	1.62	0.65
1:B:211:ARG:HH11	1:B:368:GLU:HG3	1.60	0.65
1:C:174:GLU:HG3	1:C:175:MET:H	1.62	0.65
1:C:63:GLU:N	1:C:64:PRO:HA	2.11	0.65
1:A:133:GLU:CA	1:A:134:ASP:HB2	2.23	0.65
1:B:253:CYS:SG	1:B:263:LEU:HD12	2.37	0.65
1:C:174:GLU:HG3	1:C:175:MET:N	2.11	0.65
1:C:211:ARG:HH11	1:C:368:GLU:HG3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:THR:HG21	1:E:193:LEU:HD23	1.77	0.65
1:F:23:ALA:HB1	1:F:102:VAL:HG22	1.79	0.65
1:A:148:MET:HE2	1:A:148:MET:HA	1.79	0.64
1:C:132:ARG:O	1:C:133:GLU:HG3	1.96	0.64
1:E:330:ARG:HG3	1:F:149:GLU:CG	2.24	0.64
1:A:211:ARG:HH11	1:A:368:GLU:HG3	1.62	0.64
1:C:294:PRO:CG	1:D:381:ARG:CZ	2.75	0.64
1:D:269:THR:HB	1:D:272:ASP:HB2	1.79	0.64
1:B:227:VAL:O	1:B:231:THR:HG22	1.98	0.64
1:E:23:ALA:HB1	1:E:102:VAL:HG22	1.80	0.64
1:A:66:ASP:H	1:A:69:THR:HG22	1.63	0.64
1:F:21:LEU:HD23	1:F:55:MET:HE1	1.78	0.64
1:F:211:ARG:HH11	1:F:368:GLU:HG3	1.63	0.64
1:B:104:TYR:CB	1:B:105:TYR:HB2	2.22	0.64
1:A:173:ILE:HD12	1:F:263:LEU:HD22	1.80	0.64
1:C:12:GLN:HE21	1:C:14:ILE:HG12	1.63	0.64
1:F:227:VAL:O	1:F:231:THR:HG22	1.98	0.64
1:F:63:GLU:H	1:F:64:PRO:CA	2.02	0.63
1:E:101:ASN:C	1:E:103:GLU:H	2.06	0.63
1:E:104:TYR:HA	1:E:105:TYR:CB	2.19	0.63
1:A:266:GLY:HA2	1:A:267:LYS:O	1.98	0.63
1:D:207:ILE:HD12	1:D:390:ALA:HB2	1.80	0.63
1:E:63:GLU:H	1:E:64:PRO:CA	2.05	0.63
1:C:381:ARG:HH22	1:C:388:GLN:HE22	1.47	0.63
1:D:41:GLU:HA	1:D:49:GLN:HE21	1.64	0.63
1:B:74:LEU:HD13	1:B:83:ILE:CD1	2.28	0.63
1:A:174:GLU:OE1	1:A:178:ASN:HB2	1.97	0.62
1:E:62:GLY:HA2	1:E:63:GLU:HB3	1.79	0.62
1:E:101:ASN:O	1:E:103:GLU:N	2.33	0.62
1:A:171:ASP:O	1:A:174:GLU:HG3	1.99	0.62
1:E:65:VAL:HA	1:E:69:THR:HG21	1.81	0.62
1:C:174:GLU:C	1:C:176:LEU:N	2.54	0.62
1:C:207:ILE:HD13	1:C:386:ILE:CG2	2.28	0.62
1:E:381:ARG:HH22	1:E:388:GLN:HE22	1.46	0.62
1:A:71:THR:HG22	1:A:89:LEU:HD13	1.82	0.62
1:C:174:GLU:CD	1:C:178:ASN:CB	2.73	0.62
1:E:227:VAL:O	1:E:231:THR:HG22	2.00	0.62
1:C:307:ARG:NE	1:D:36:GLU:CD	2.58	0.62
1:D:133:GLU:CA	1:D:134:ASP:HB2	2.30	0.62
1:E:28:PRO:C	1:E:30:ALA:H	2.08	0.62
1:D:188:THR:HG21	1:D:193:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:H	1:A:134:ASP:HB2	0.55	0.61
1:C:23:ALA:HB1	1:C:102:VAL:HG22	1.83	0.61
1:E:19:ALA:O	1:E:23:ALA:HB2	2.00	0.61
1:E:47:ALA:HB1	1:E:83:ILE:HG23	1.82	0.61
1:F:62:GLY:HA2	1:F:63:GLU:HB3	1.82	0.61
1:C:147:ILE:HG22	1:C:147:ILE:O	1.98	0.61
1:C:147:ILE:O	1:C:147:ILE:CG2	2.48	0.61
1:D:296:ILE:CG2	1:D:300:ASP:HB2	2.31	0.61
1:A:296:ILE:CG2	1:A:300:ASP:HB2	2.30	0.61
1:F:267:LYS:O	1:F:268:LEU:HB2	2.01	0.60
1:A:32:VAL:HB	1:A:33:PRO:HD3	1.82	0.60
1:B:39:ILE:HB	1:B:40:PRO:HD2	1.84	0.60
1:C:296:ILE:HG22	1:C:300:ASP:HB2	1.83	0.60
1:A:198:SER:H	1:A:199:GLY:HA2	1.66	0.60
1:A:296:ILE:HG22	1:A:300:ASP:HB2	1.83	0.60
1:A:306:ARG:NH2	1:B:103:GLU:CD	2.59	0.60
1:A:162:ILE:O	1:A:164:ASP:N	2.35	0.60
1:D:266:GLY:HA2	1:D:267:LYS:O	2.02	0.60
1:A:67:LEU:O	1:A:71:THR:HG23	2.02	0.60
1:C:133:GLU:CA	1:C:134:ASP:HB2	2.27	0.60
1:C:171:ASP:O	1:C:175:MET:CG	2.48	0.60
1:B:63:GLU:N	1:B:64:PRO:HA	2.14	0.59
1:C:412:ILE:HG21	1:C:438:PHE:HE2	1.66	0.59
1:C:412:ILE:HG21	1:C:438:PHE:CE2	2.37	0.59
1:D:52:PHE:HA	1:D:55:MET:HE2	1.84	0.59
1:A:246:GLN:HE22	1:B:420:ARG:HB3	1.65	0.59
1:F:62:GLY:CA	1:F:63:GLU:HB3	2.32	0.59
1:C:294:PRO:CB	1:D:381:ARG:CD	2.78	0.59
1:D:135:GLU:HG2	1:D:330:ARG:CZ	2.32	0.59
1:D:296:ILE:HG22	1:D:300:ASP:HB2	1.82	0.59
1:F:28:PRO:C	1:F:30:ALA:H	2.09	0.59
1:F:188:THR:HG21	1:F:193:LEU:HD23	1.83	0.59
1:C:174:GLU:CD	1:C:178:ASN:HB3	2.26	0.59
1:B:50:LYS:NZ	1:B:82:GLU:OE2	2.36	0.59
1:A:377:MET:HE3	1:A:387:GLU:HG3	1.84	0.59
1:C:103:GLU:N	1:C:104:TYR:HB2	2.17	0.59
1:D:135:GLU:CG	1:D:330:ARG:NH2	2.55	0.59
1:D:62:GLY:CA	1:D:63:GLU:CB	2.76	0.59
1:F:296:ILE:CG2	1:F:300:ASP:HB2	2.33	0.58
1:A:61:ARG:CB	1:A:62:GLY:CA	2.79	0.58
1:B:25:PHE:HZ	1:B:89:LEU:HD22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ARG:HH22	1:B:388:GLN:HE22	1.51	0.58
1:D:207:ILE:HD13	1:D:386:ILE:HG22	1.83	0.58
1:F:412:ILE:HG21	1:F:438:PHE:CE2	2.38	0.58
1:B:66:ASP:H	1:B:69:THR:HG22	1.69	0.58
1:C:75:ALA:HB2	1:C:80:LEU:HD12	1.85	0.58
1:F:296:ILE:HG22	1:F:300:ASP:HB2	1.84	0.58
1:A:297:ARG:NH2	1:A:329:GLY:O	2.36	0.58
1:A:104:TYR:CG	1:B:63:GLU:O	2.57	0.58
1:A:412:ILE:HG21	1:A:438:PHE:HE2	1.69	0.58
1:F:233:GLU:CG	1:F:315:GLY:HA3	2.34	0.58
1:E:321:TYR:H	1:E:360:LEU:HB2	1.69	0.58
1:B:133:GLU:CA	1:B:134:ASP:HB2	2.32	0.57
1:B:24:VAL:O	1:B:28:PRO:HB3	2.04	0.57
1:E:266:GLY:HA2	1:E:267:LYS:O	2.04	0.57
1:E:412:ILE:HG21	1:E:438:PHE:HE2	1.70	0.57
1:A:30:ALA:O	1:A:33:PRO:HD2	2.03	0.57
1:A:378:SER:O	1:A:382:GLU:HG2	2.04	0.57
1:B:314:LEU:HD23	1:B:315:GLY:N	2.20	0.57
1:C:296:ILE:CG2	1:C:300:ASP:HB2	2.34	0.57
1:D:104:TYR:CB	1:D:105:TYR:HB2	2.32	0.56
1:A:412:ILE:HG21	1:A:438:PHE:CE2	2.39	0.56
1:D:141:ASP:C	1:D:328:SER:HB2	2.30	0.56
1:B:412:ILE:HG21	1:B:438:PHE:HE2	1.69	0.56
1:C:104:TYR:H	1:C:107:ARG:H	1.53	0.56
1:C:269:THR:HB	1:C:272:ASP:HB2	1.86	0.56
1:A:162:ILE:HD13	1:F:288:ILE:HB	1.86	0.56
1:F:133:GLU:CA	1:F:134:ASP:HB2	2.32	0.56
1:C:40:PRO:HG2	1:C:53:HIS:HD2	1.71	0.56
1:C:103:GLU:N	1:C:104:TYR:CB	2.69	0.56
1:A:246:GLN:HE22	1:B:420:ARG:CB	2.18	0.56
1:B:233:GLU:HG2	1:B:315:GLY:HA3	1.89	0.56
1:D:51:ILE:HD11	1:D:83:ILE:HG21	1.87	0.56
1:B:296:ILE:CG2	1:B:300:ASP:HB2	2.36	0.55
1:C:302:ARG:HH12	1:D:60:ASP:HA	1.70	0.55
1:D:148:MET:HE2	1:D:148:MET:HA	1.88	0.55
1:A:105:TYR:OH	1:B:66:ASP:OD2	2.24	0.55
1:B:207:ILE:CD1	1:B:386:ILE:HG22	2.36	0.55
1:C:32:VAL:HB	1:C:33:PRO:HD3	1.88	0.55
1:A:231:THR:HG23	1:A:233:GLU:H	1.71	0.55
1:B:45:ARG:O	1:B:46:ALA:C	2.50	0.55
1:B:296:ILE:HG22	1:B:300:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:GLU:H	1:D:134:ASP:HB3	1.62	0.55
1:E:296:ILE:HG22	1:E:300:ASP:HB2	1.89	0.55
1:E:412:ILE:HG21	1:E:438:PHE:CE2	2.42	0.55
1:B:208:VAL:HB	1:B:360:LEU:HD23	1.87	0.55
1:B:268:LEU:CB	1:C:177:HIS:HE1	2.07	0.55
1:F:66:ASP:OD1	1:F:66:ASP:C	2.48	0.55
1:B:262:ASN:OD1	1:B:268:LEU:HG	2.07	0.55
1:C:21:LEU:HB3	1:C:92:LEU:HD13	1.88	0.55
1:F:316:MET:HG2	1:F:356:PRO:HG2	1.88	0.55
1:A:302:ARG:CG	1:A:349:LEU:HD13	2.37	0.54
1:A:41:GLU:OE1	1:A:41:GLU:N	2.34	0.54
1:B:228:ALA:HB1	1:B:286:ALA:HB1	1.89	0.54
1:A:175:MET:O	1:A:179:ARG:HD2	2.06	0.54
1:E:302:ARG:HG2	1:E:349:LEU:HD13	1.89	0.54
1:A:292:ASP:O	1:B:351:ARG:CD	2.56	0.54
1:C:104:TYR:HD1	1:C:105:TYR:CG	2.26	0.54
1:B:132:ARG:NH1	1:B:135:GLU:OE1	2.39	0.54
1:F:381:ARG:HH22	1:F:388:GLN:HE22	1.55	0.54
1:E:105:TYR:HE2	1:F:68:VAL:HB	1.71	0.54
1:A:294:PRO:HD3	1:B:351:ARG:HD2	1.89	0.53
1:E:104:TYR:CD1	1:E:104:TYR:C	2.84	0.53
1:A:245:GLN:HE22	1:B:202:ARG:NH1	2.06	0.53
1:D:104:TYR:HB3	1:D:105:TYR:CB	2.35	0.53
1:F:196:MET:HE3	1:F:423:PRO:HB2	1.89	0.53
1:C:294:PRO:HB2	1:D:381:ARG:CG	2.38	0.53
1:D:207:ILE:CD1	1:D:390:ALA:HB2	2.38	0.53
1:A:64:PRO:O	1:A:69:THR:HG21	2.08	0.53
1:A:161:ASN:O	1:A:162:ILE:C	2.52	0.53
1:E:133:GLU:CA	1:E:134:ASP:HB2	2.33	0.53
1:C:144:ASP:O	1:C:145:ARG:C	2.51	0.53
1:D:145:ARG:CD	1:D:328:SER:OG	2.52	0.53
1:C:231:THR:HG23	1:C:233:GLU:H	1.74	0.53
1:E:62:GLY:CA	1:E:63:GLU:HB3	2.39	0.53
1:A:262:ASN:HD21	1:A:268:LEU:HA	1.74	0.53
1:A:314:LEU:HD23	1:A:315:GLY:N	2.23	0.53
1:B:30:ALA:HB1	1:B:102:VAL:HG21	1.90	0.53
1:D:381:ARG:HH22	1:D:388:GLN:HE22	1.56	0.53
1:B:267:LYS:O	1:B:268:LEU:HB2	2.08	0.53
1:E:269:THR:HB	1:E:272:ASP:HB2	1.90	0.53
1:F:52:PHE:HA	1:F:55:MET:HE2	1.90	0.53
1:F:62:GLY:CA	1:F:63:GLU:CB	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:PRO:C	1:D:30:ALA:H	2.16	0.53
1:E:296:ILE:CG2	1:E:300:ASP:HB2	2.39	0.53
1:F:233:GLU:HG2	1:F:315:GLY:HA3	1.90	0.53
1:A:302:ARG:HG2	1:A:349:LEU:HD13	1.91	0.52
1:B:12:GLN:HE21	1:B:14:ILE:HG12	1.74	0.52
1:B:105:TYR:O	1:B:109:VAL:HG23	2.10	0.52
1:C:104:TYR:HE2	1:D:63:GLU:HB2	1.75	0.52
1:D:71:THR:HG22	1:D:89:LEU:HD13	1.90	0.52
1:D:228:ALA:HB1	1:D:286:ALA:HB1	1.91	0.52
1:B:320:ASP:HA	1:B:360:LEU:HD12	1.90	0.52
1:B:412:ILE:HG21	1:B:438:PHE:CE2	2.44	0.52
1:A:166:LEU:HD22	1:F:280:MET:HG2	1.91	0.52
1:C:294:PRO:HB2	1:D:381:ARG:HE	1.63	0.52
1:D:61:ARG:CB	1:D:62:GLY:CA	2.87	0.52
1:B:302:ARG:NH2	1:B:348:ALA:HB1	2.24	0.52
1:E:330:ARG:CZ	1:F:149:GLU:HA	2.39	0.52
1:A:160:LYS:HB3	1:F:290:ILE:O	2.09	0.52
1:C:348:ALA:HB2	1:D:61:ARG:O	2.10	0.52
1:F:104:TYR:HB3	1:F:105:TYR:CB	2.35	0.52
1:F:104:TYR:CB	1:F:105:TYR:HB2	2.38	0.52
1:E:207:ILE:HD13	1:E:386:ILE:CG2	2.38	0.52
1:F:148:MET:O	1:F:149:GLU:HG3	2.10	0.52
1:E:265:THR:HB	1:E:267:LYS:HD2	1.92	0.52
1:E:265:THR:CG2	1:F:423:PRO:HB3	2.33	0.52
1:F:227:VAL:HG21	1:F:316:MET:HE2	1.91	0.52
1:B:392:ILE:HA	1:B:418:LYS:O	2.10	0.52
1:D:211:ARG:HH11	1:D:368:GLU:HG3	1.75	0.52
1:C:161:ASN:ND2	1:C:163:LYS:HG2	2.25	0.52
1:E:267:LYS:O	1:E:268:LEU:HB2	2.09	0.52
1:F:197:THR:O	1:F:198:SER:HB2	2.10	0.52
1:B:28:PRO:C	1:B:30:ALA:H	2.16	0.51
1:A:104:TYR:CD2	1:B:63:GLU:O	2.62	0.51
1:B:104:TYR:HA	1:B:106:ALA:H	1.75	0.51
1:C:348:ALA:CB	1:D:61:ARG:O	2.58	0.51
1:E:83:ILE:HG22	1:E:84:GLY:H	1.76	0.51
1:D:31:LEU:HD22	1:D:65:VAL:HG21	1.93	0.51
1:F:105:TYR:O	1:F:109:VAL:HG23	2.10	0.51
1:D:197:THR:O	1:D:198:SER:HB2	2.11	0.51
1:B:269:THR:HB	1:B:272:ASP:HB2	1.93	0.51
1:C:63:GLU:H	1:C:64:PRO:CA	2.21	0.51
1:F:12:GLN:HE21	1:F:14:ILE:HD11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HG22	1:A:163:LYS:N	2.25	0.51
1:C:174:GLU:OE1	1:C:178:ASN:ND2	2.33	0.51
1:A:162:ILE:O	1:A:165:ILE:N	2.44	0.51
1:C:174:GLU:C	1:C:177:HIS:H	1.99	0.51
1:E:51:ILE:HD11	1:E:83:ILE:HG21	1.92	0.51
1:E:61:ARG:CB	1:E:62:GLY:CA	2.87	0.51
1:B:266:GLY:HA2	1:B:267:LYS:O	2.11	0.50
1:F:71:THR:HG22	1:F:89:LEU:HD12	1.93	0.50
1:A:173:ILE:O	1:A:173:ILE:HG22	2.11	0.50
1:B:25:PHE:CZ	1:B:89:LEU:HD22	2.46	0.50
1:B:74:LEU:HD13	1:B:83:ILE:HD11	1.93	0.50
1:C:74:LEU:HD22	1:C:83:ILE:HD11	1.93	0.50
1:E:103:GLU:N	1:E:104:TYR:HB2	2.26	0.50
1:E:321:TYR:HA	1:E:360:LEU:O	2.12	0.50
1:A:378:SER:CB	1:F:241:GLU:HG3	2.40	0.50
1:B:135:GLU:HB3	1:B:138:VAL:HB	1.94	0.50
1:C:50:LYS:NZ	1:C:82:GLU:OE2	2.32	0.50
1:D:262:ASN:HD21	1:D:268:LEU:HA	1.75	0.50
1:B:216:LYS:HB2	1:B:360:LEU:HD22	1.93	0.50
1:D:32:VAL:HB	1:D:33:PRO:CD	2.36	0.50
1:D:412:ILE:HG21	1:D:438:PHE:HE2	1.76	0.50
1:B:133:GLU:N	1:B:134:ASP:CB	2.33	0.50
1:B:280:MET:SD	1:C:170:TYR:CD1	3.04	0.50
1:D:265:THR:O	1:D:265:THR:HG22	2.11	0.50
1:F:76:ALA:C	1:F:78:GLU:H	2.20	0.50
1:A:128:ASP:HB3	1:A:139:LEU:HD21	1.92	0.50
1:A:321:TYR:CE1	1:A:324:LEU:HG	2.47	0.50
1:B:378:SER:O	1:B:382:GLU:HG2	2.12	0.50
1:C:175:MET:O	1:C:179:ARG:HD3	2.12	0.50
1:A:294:PRO:HA	1:B:351:ARG:HH12	1.77	0.49
1:A:294:PRO:CA	1:B:351:ARG:NH1	2.74	0.49
1:E:290:ILE:O	1:F:160:LYS:HB3	2.12	0.49
1:A:162:ILE:HG23	1:A:166:LEU:HD12	1.94	0.49
1:D:412:ILE:HG21	1:D:438:PHE:CE2	2.47	0.49
1:C:66:ASP:H	1:C:69:THR:HG22	1.77	0.49
1:C:241:GLU:HG3	1:D:378:SER:CB	2.40	0.49
1:A:58:VAL:HG13	1:A:63:GLU:HG2	1.95	0.49
1:C:174:GLU:CD	1:C:178:ASN:HB2	2.37	0.49
1:E:74:LEU:HD22	1:E:83:ILE:HD11	1.94	0.49
1:D:38:LEU:HD11	1:D:106:ALA:HA	1.93	0.49
1:D:61:ARG:HB2	1:D:62:GLY:CA	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:TYR:OH	1:F:63:GLU:HB2	2.11	0.49
1:E:377:MET:HE3	1:E:387:GLU:HG3	1.95	0.49
1:F:74:LEU:HD13	1:F:83:ILE:CD1	2.42	0.49
1:F:259:ASN:O	1:F:262:ASN:HB3	2.12	0.49
1:C:266:GLY:HA2	1:C:267:LYS:O	2.13	0.49
1:E:198:SER:H	1:E:199:GLY:HA2	1.76	0.49
1:C:197:THR:O	1:C:198:SER:HB2	2.12	0.49
1:D:234:ASN:HB2	1:D:313:GLY:O	2.13	0.49
1:F:378:SER:O	1:F:382:GLU:HG2	2.13	0.49
1:A:28:PRO:C	1:A:30:ALA:H	2.20	0.49
1:A:414:ILE:HD11	1:A:429:LEU:HD12	1.95	0.49
1:D:231:THR:HG23	1:D:233:GLU:H	1.78	0.49
1:D:314:LEU:HD23	1:D:315:GLY:N	2.27	0.49
1:B:212:PRO:O	1:B:213:SER:HB2	2.13	0.48
1:A:302:ARG:O	1:A:306:ARG:HB2	2.13	0.48
1:C:51:ILE:HD11	1:C:83:ILE:HG21	1.94	0.48
1:A:134:ASP:O	1:A:135:GLU:HG3	2.13	0.48
1:C:71:THR:HG22	1:C:89:LEU:HD13	1.96	0.48
1:F:147:ILE:O	1:F:147:ILE:CG2	2.61	0.48
1:F:233:GLU:HG3	1:F:315:GLY:HA3	1.96	0.48
1:B:68:VAL:HG12	1:B:69:THR:N	2.28	0.48
1:B:273:TRP:HZ3	1:C:177:HIS:ND1	2.11	0.48
1:A:263:LEU:HD23	1:A:268:LEU:HD11	1.96	0.48
1:C:267:LYS:O	1:C:268:LEU:HB2	2.12	0.48
1:C:378:SER:O	1:C:382:GLU:HG2	2.13	0.48
1:A:294:PRO:HG3	1:B:348:ALA:CB	2.44	0.48
1:D:23:ALA:HB1	1:D:102:VAL:HG22	1.94	0.48
1:D:135:GLU:HB3	1:D:138:VAL:HB	1.95	0.48
1:E:30:ALA:O	1:E:33:PRO:HD2	2.13	0.48
1:E:101:ASN:C	1:E:103:GLU:N	2.72	0.48
1:E:316:MET:HG2	1:E:356:PRO:HG2	1.96	0.48
1:F:101:ASN:HB3	1:F:105:TYR:CD1	2.48	0.48
1:B:132:ARG:HD2	1:B:139:LEU:HG	1.95	0.48
1:E:66:ASP:H	1:E:69:THR:CG2	2.21	0.48
1:B:297:ARG:NH2	1:B:329:GLY:O	2.47	0.48
1:D:53:HIS:HE1	1:D:57:ARG:NH1	2.11	0.48
1:A:104:TYR:O	1:A:108:ILE:HG12	2.14	0.48
1:D:262:ASN:OD1	1:D:268:LEU:HG	2.14	0.48
1:A:160:LYS:CB	1:F:290:ILE:O	2.62	0.48
1:C:28:PRO:C	1:C:30:ALA:N	2.63	0.48
1:C:302:ARG:NH1	1:D:59:ALA:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:LEU:HD23	1:D:268:LEU:HD11	1.95	0.48
1:D:316:MET:HG2	1:D:356:PRO:HG2	1.96	0.48
1:D:314:LEU:HD21	1:D:317:ILE:HG13	1.96	0.47
1:E:414:ILE:HD11	1:E:429:LEU:HD12	1.96	0.47
1:F:184:THR:N	1:F:198:SER:O	2.47	0.47
1:A:179:ARG:O	1:A:180:ASP:C	2.57	0.47
1:D:33:PRO:HA	1:D:36:GLU:OE2	2.14	0.47
1:D:50:LYS:NZ	1:D:82:GLU:OE2	2.46	0.47
1:E:211:ARG:HH11	1:E:368:GLU:HG3	1.79	0.47
1:E:268:LEU:HD13	1:E:273:TRP:CE3	2.50	0.47
1:A:296:ILE:HG22	1:A:297:ARG:O	2.14	0.47
1:C:102:VAL:H	1:C:105:TYR:HD1	1.63	0.47
1:E:259:ASN:O	1:E:262:ASN:HB3	2.15	0.47
1:B:62:GLY:HA2	1:B:63:GLU:HA	1.59	0.47
1:D:268:LEU:HD13	1:D:273:TRP:CE3	2.49	0.47
1:A:12:GLN:HE21	1:A:14:ILE:HG12	1.80	0.47
1:C:161:ASN:HD22	1:C:163:LYS:HG2	1.80	0.47
1:D:267:LYS:O	1:D:268:LEU:HB2	2.14	0.47
1:A:86:VAL:HA	1:A:89:LEU:HD12	1.97	0.47
1:A:206:ILE:HA	1:A:392:ILE:HG23	1.97	0.47
1:B:263:LEU:HD23	1:B:268:LEU:HD11	1.95	0.47
1:B:439:VAL:HG12	1:B:440:ASN:N	2.29	0.47
1:D:141:ASP:C	1:D:143:ALA:N	2.69	0.47
1:E:233:GLU:HG2	1:E:315:GLY:HA3	1.97	0.47
1:A:233:GLU:CG	1:A:315:GLY:HA3	2.44	0.47
1:C:234:ASN:HB2	1:C:313:GLY:O	2.15	0.47
1:D:216:LYS:HB2	1:D:360:LEU:HD22	1.96	0.47
1:A:174:GLU:OE2	1:A:175:MET:HG2	2.15	0.47
1:B:145:ARG:HD2	1:B:330:ARG:CZ	2.45	0.47
1:C:61:ARG:HD3	1:C:63:GLU:CD	2.40	0.47
1:D:198:SER:H	1:D:199:GLY:HA2	1.75	0.47
1:F:19:ALA:O	1:F:23:ALA:HB2	2.15	0.47
1:C:13:SER:O	1:C:14:ILE:C	2.59	0.46
1:C:293:THR:HA	1:C:294:PRO:HD2	1.54	0.46
1:B:102:VAL:O	1:B:105:TYR:HB2	2.15	0.46
1:E:10:PRO:HA	1:E:11:PRO:HD2	1.77	0.46
1:E:24:VAL:HG11	1:E:55:MET:SD	2.55	0.46
1:F:28:PRO:C	1:F:30:ALA:N	2.72	0.46
1:C:219:PHE:CE2	1:C:223:ILE:HD11	2.50	0.46
1:C:302:ARG:NH1	1:D:60:ASP:HA	2.30	0.46
1:E:207:ILE:CD1	1:E:386:ILE:HG22	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ILE:CD1	1:C:45:ARG:HG3	2.45	0.46
1:D:136:ILE:C	1:D:138:VAL:H	2.24	0.46
1:A:198:SER:N	1:A:199:GLY:CA	2.75	0.46
1:A:416:ILE:O	1:A:424:VAL:HG13	2.15	0.46
1:D:61:ARG:HD3	1:D:63:GLU:OE2	2.16	0.46
1:D:208:VAL:HB	1:D:360:LEU:HD23	1.98	0.46
1:E:245:GLN:NE2	1:F:168:GLN:OE1	2.48	0.46
1:F:207:ILE:HD12	1:F:390:ALA:CB	2.34	0.46
1:F:377:MET:HE3	1:F:387:GLU:HG3	1.98	0.46
1:C:174:GLU:C	1:C:176:LEU:H	2.24	0.46
1:E:197:THR:O	1:E:198:SER:HB2	2.15	0.46
1:F:32:VAL:HB	1:F:33:PRO:CD	2.39	0.46
1:A:63:GLU:N	1:A:64:PRO:HA	2.28	0.46
1:D:64:PRO:HB2	1:D:65:VAL:H	1.59	0.46
1:D:74:LEU:HD22	1:D:83:ILE:HD11	1.98	0.46
1:E:216:LYS:HB2	1:E:360:LEU:HD22	1.97	0.45
1:F:74:LEU:HD13	1:F:83:ILE:HD11	1.98	0.45
1:E:233:GLU:CG	1:E:315:GLY:HA3	2.46	0.45
1:F:207:ILE:CD1	1:F:390:ALA:HB2	2.33	0.45
1:A:168:GLN:O	1:A:170:TYR:N	2.49	0.45
1:D:47:ALA:HB1	1:D:83:ILE:HG23	1.97	0.45
1:E:101:ASN:HB2	1:E:105:TYR:CE1	2.51	0.45
1:B:11:PRO:HG2	1:B:116:ARG:HG2	1.97	0.45
1:C:184:THR:N	1:C:198:SER:O	2.50	0.45
1:D:273:TRP:CH2	1:E:173:ILE:CG2	2.98	0.45
1:E:302:ARG:O	1:E:306:ARG:HB2	2.16	0.45
1:F:135:GLU:HB3	1:F:138:VAL:HB	1.97	0.45
1:A:25:PHE:HZ	1:A:89:LEU:HD22	1.82	0.45
1:A:176:LEU:HB2	1:A:177:HIS:HD2	1.81	0.45
1:B:263:LEU:HD22	1:C:173:ILE:HG23	1.99	0.45
1:B:102:VAL:O	1:B:105:TYR:CB	2.64	0.45
1:B:202:ARG:HA	1:B:356:PRO:HD3	1.99	0.45
1:C:268:LEU:HD13	1:C:273:TRP:CE3	2.51	0.45
1:D:32:VAL:CB	1:D:33:PRO:HD3	2.41	0.45
1:F:24:VAL:HG11	1:F:55:MET:SD	2.57	0.45
1:A:53:HIS:HE1	1:A:57:ARG:HH11	1.62	0.45
1:A:168:GLN:C	1:A:170:TYR:N	2.75	0.45
1:A:169:THR:O	1:A:169:THR:HG22	2.17	0.45
1:D:321:TYR:CZ	1:D:324:LEU:HG	2.52	0.45
1:E:208:VAL:HB	1:E:360:LEU:HD23	1.98	0.45
1:B:363:LEU:HD23	1:B:380:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:VAL:HA	1:C:89:LEU:HD12	1.99	0.45
1:D:53:HIS:CE1	1:D:57:ARG:HH11	2.35	0.45
1:E:163:LYS:HG3	1:E:164:ASP:N	2.32	0.45
1:E:268:LEU:HD13	1:E:273:TRP:CZ3	2.52	0.45
1:B:105:TYR:HD2	1:B:105:TYR:HA	1.71	0.45
1:B:386:ILE:H	1:B:386:ILE:HG13	1.44	0.45
1:E:234:ASN:HB2	1:E:313:GLY:O	2.16	0.45
1:E:262:ASN:HD21	1:E:268:LEU:HA	1.82	0.45
1:F:132:ARG:NH1	1:F:135:GLU:OE1	2.50	0.45
1:B:347:LYS:HE3	1:B:351:ARG:NH2	2.32	0.44
1:C:71:THR:HG22	1:C:89:LEU:CD1	2.47	0.44
1:C:97:PRO:HD2	1:C:98:THR:HG22	1.99	0.44
1:B:269:THR:CB	1:B:272:ASP:HB2	2.47	0.44
1:C:110:GLU:O	1:C:114:VAL:HG23	2.16	0.44
1:C:206:ILE:HA	1:C:392:ILE:HG23	1.98	0.44
1:C:302:ARG:O	1:C:306:ARG:HB2	2.17	0.44
1:D:416:ILE:O	1:D:424:VAL:HG13	2.16	0.44
1:F:24:VAL:HA	1:F:30:ALA:HB3	2.00	0.44
1:A:45:ARG:O	1:A:46:ALA:C	2.60	0.44
1:A:381:ARG:HH22	1:A:388:GLN:NE2	2.09	0.44
1:C:30:ALA:HB1	1:C:102:VAL:HG21	1.99	0.44
1:E:99:ALA:O	1:E:102:VAL:HG23	2.17	0.44
1:A:192:GLU:HB3	1:A:427:VAL:CG1	2.48	0.44
1:A:15:GLU:OE2	1:B:86:VAL:HG11	2.17	0.44
1:B:48:HIS:O	1:B:49:GLN:C	2.59	0.44
1:B:414:ILE:HD11	1:B:429:LEU:HD12	2.00	0.44
1:D:302:ARG:O	1:D:306:ARG:HB2	2.17	0.44
1:E:314:LEU:HD23	1:E:315:GLY:N	2.32	0.44
1:A:11:PRO:HG3	1:A:119:ILE:CD1	2.47	0.44
1:C:294:PRO:HB2	1:D:381:ARG:HG2	2.00	0.44
1:A:159:PHE:HD1	1:A:160:LYS:N	2.13	0.44
1:A:200:PHE:HE2	1:A:223:ILE:HD13	1.82	0.44
1:A:411:ILE:HD11	1:A:441:LEU:HD21	1.99	0.44
1:B:262:ASN:HD21	1:B:268:LEU:HA	1.82	0.44
1:C:24:VAL:HG21	1:C:55:MET:HE3	1.99	0.44
1:C:307:ARG:NE	1:D:36:GLU:OE2	2.50	0.44
1:C:321:TYR:H	1:C:360:LEU:HB2	1.83	0.44
1:A:246:GLN:NE2	1:B:420:ARG:CB	2.70	0.44
1:F:268:LEU:HD13	1:F:273:TRP:CE3	2.52	0.44
1:B:145:ARG:HD2	1:B:330:ARG:NH2	2.33	0.43
1:C:63:GLU:N	1:C:64:PRO:CA	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:HG22	1:D:297:ARG:NH1	2.33	0.43
1:F:262:ASN:O	1:F:266:GLY:HA2	2.18	0.43
1:F:267:LYS:O	1:F:268:LEU:CB	2.65	0.43
1:B:32:VAL:HB	1:B:33:PRO:HD3	2.00	0.43
1:C:40:PRO:HG2	1:C:53:HIS:CD2	2.52	0.43
1:D:210:ALA:HB3	1:D:216:LYS:HB3	1.99	0.43
1:E:132:ARG:HD2	1:E:139:LEU:HG	2.00	0.43
1:E:314:LEU:HD21	1:E:317:ILE:HG13	2.00	0.43
1:B:11:PRO:HG2	1:B:116:ARG:CG	2.47	0.43
1:D:134:ASP:C	1:D:135:GLU:HG3	2.43	0.43
1:B:231:THR:HG23	1:B:233:GLU:H	1.83	0.43
1:D:212:PRO:O	1:D:213:SER:HB2	2.18	0.43
1:D:321:TYR:CE1	1:D:324:LEU:HG	2.53	0.43
1:F:53:HIS:HE1	1:F:57:ARG:NH1	2.17	0.43
1:B:66:ASP:C	1:B:66:ASP:OD1	2.62	0.43
1:B:188:THR:HG23	1:B:223:ILE:HG23	2.00	0.43
1:B:268:LEU:HD13	1:B:273:TRP:CE3	2.53	0.43
1:B:268:LEU:CD1	1:C:177:HIS:CE1	2.98	0.43
1:B:347:LYS:HG3	1:B:351:ARG:NH1	2.33	0.43
1:C:74:LEU:HD13	1:C:83:ILE:HD11	2.01	0.43
1:D:280:MET:HG2	1:E:166:LEU:HD22	2.01	0.43
1:E:19:ALA:O	1:E:23:ALA:CB	2.65	0.43
1:A:55:MET:HG3	1:A:65:VAL:HG11	2.01	0.43
1:A:268:LEU:HD13	1:A:273:TRP:CZ3	2.54	0.43
1:B:99:ALA:O	1:B:102:VAL:HG23	2.19	0.43
1:D:136:ILE:C	1:D:138:VAL:N	2.76	0.43
1:F:208:VAL:HB	1:F:360:LEU:HD23	2.01	0.43
1:F:293:THR:HA	1:F:294:PRO:HD2	1.81	0.43
1:A:168:GLN:C	1:A:170:TYR:H	2.27	0.43
1:A:302:ARG:HG3	1:A:349:LEU:HD13	2.01	0.43
1:B:61:ARG:CB	1:B:62:GLY:CA	2.93	0.43
1:C:210:ALA:HB3	1:C:216:LYS:HB3	2.00	0.43
1:D:14:ILE:HD13	1:D:14:ILE:HA	1.90	0.43
1:A:259:ASN:O	1:A:262:ASN:HB3	2.19	0.43
1:B:188:THR:HG21	1:B:193:LEU:HD23	2.00	0.43
1:C:233:GLU:HG2	1:C:315:GLY:HA3	2.00	0.43
1:C:321:TYR:CE1	1:C:324:LEU:HG	2.54	0.43
1:D:45:ARG:O	1:D:46:ALA:C	2.61	0.43
1:E:104:TYR:OH	1:F:63:GLU:CG	2.67	0.43
1:E:253:CYS:SG	1:E:263:LEU:HD12	2.59	0.43
1:F:74:LEU:HD22	1:F:83:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:VAL:HG12	1:F:440:ASN:N	2.34	0.43
1:C:61:ARG:CB	1:C:62:GLY:CA	2.84	0.43
1:D:39:ILE:O	1:D:41:GLU:N	2.52	0.43
1:D:381:ARG:C	1:D:383:SER:H	2.27	0.43
1:F:13:SER:O	1:F:14:ILE:C	2.62	0.43
1:F:308:LEU:HD23	1:F:314:LEU:HD12	1.99	0.43
1:D:148:MET:O	1:D:149:GLU:HG3	2.19	0.42
1:D:209:ALA:HA	1:D:361:SER:O	2.19	0.42
1:E:148:MET:O	1:E:149:GLU:HG3	2.18	0.42
1:E:293:THR:HB	1:E:296:ILE:HG12	2.00	0.42
1:B:321:TYR:CZ	1:B:324:LEU:HG	2.55	0.42
1:C:62:GLY:HA2	1:C:63:GLU:HA	1.83	0.42
1:C:212:PRO:O	1:C:213:SER:HB2	2.17	0.42
1:B:96:VAL:HA	1:B:97:PRO:HD3	1.91	0.42
1:B:240:LEU:HD22	1:B:293:THR:O	2.18	0.42
1:B:273:TRP:HZ3	1:C:177:HIS:CE1	2.37	0.42
1:D:66:ASP:N	1:D:69:THR:HG22	2.28	0.42
1:D:69:THR:HG23	1:D:70:VAL:N	2.34	0.42
1:E:71:THR:HA	1:E:74:LEU:HD12	2.02	0.42
1:F:53:HIS:CE1	1:F:57:ARG:HH11	2.37	0.42
1:F:266:GLY:HA2	1:F:267:LYS:O	2.20	0.42
1:A:19:ALA:O	1:A:20:VAL:C	2.61	0.42
1:A:161:ASN:CG	1:A:163:LYS:HG2	2.45	0.42
1:C:265:THR:HB	1:C:267:LYS:HD2	2.02	0.42
1:D:135:GLU:HG2	1:D:330:ARG:NE	2.35	0.42
1:D:378:SER:O	1:D:382:GLU:HG2	2.19	0.42
1:A:161:ASN:O	1:A:163:LYS:N	2.52	0.42
1:A:185:GLY:HA3	1:A:201:GLN:HG2	2.02	0.42
1:A:210:ALA:HB2	1:A:396:LEU:HB2	2.01	0.42
1:C:103:GLU:H	1:C:104:TYR:HB2	1.84	0.42
1:F:32:VAL:CB	1:F:33:PRO:HD3	2.39	0.42
1:C:96:VAL:HA	1:C:97:PRO:HD3	1.83	0.42
1:C:115:LEU:C	1:C:117:ARG:H	2.28	0.42
1:C:314:LEU:HD21	1:C:317:ILE:HG13	2.02	0.42
1:D:196:MET:HE1	1:D:425:GLY:N	2.34	0.42
1:E:161:ASN:OD1	1:E:162:ILE:N	2.53	0.42
1:B:76:ALA:HA	1:F:133:GLU:HB3	2.00	0.42
1:C:14:ILE:HD11	1:C:45:ARG:HG3	2.02	0.42
1:D:24:VAL:HG13	1:D:31:LEU:HB2	2.01	0.42
1:D:53:HIS:HE1	1:D:57:ARG:HH11	1.68	0.42
1:F:198:SER:H	1:F:199:GLY:HA2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HD3	1:A:135:GLU:OE1	2.20	0.42
1:B:51:ILE:C	1:B:53:HIS:N	2.78	0.42
1:B:65:VAL:HA	1:B:69:THR:HG21	2.02	0.42
1:B:302:ARG:O	1:B:306:ARG:HB2	2.20	0.42
1:C:74:LEU:HD13	1:C:83:ILE:CD1	2.50	0.42
1:C:179:ARG:NE	1:C:179:ARG:HA	2.35	0.42
1:D:388:GLN:HE21	1:D:388:GLN:HB2	1.57	0.42
1:E:267:LYS:O	1:E:268:LEU:CB	2.68	0.42
1:E:378:SER:O	1:E:382:GLU:HG2	2.20	0.42
1:A:259:ASN:HB3	1:A:262:ASN:HB3	2.01	0.41
1:A:347:LYS:HE3	1:A:351:ARG:CZ	2.50	0.41
1:B:64:PRO:O	1:B:69:THR:HG21	2.20	0.41
1:A:48:HIS:O	1:A:49:GLN:C	2.63	0.41
1:A:188:THR:OG1	1:A:194:ASP:OD1	2.32	0.41
1:B:10:PRO:HA	1:B:11:PRO:HD2	1.86	0.41
1:B:263:LEU:CD2	1:B:268:LEU:HD11	2.50	0.41
1:C:267:LYS:O	1:C:268:LEU:CB	2.67	0.41
1:E:192:GLU:HB3	1:E:427:VAL:HG13	2.02	0.41
1:F:207:ILE:CD1	1:F:386:ILE:HG22	2.46	0.41
1:A:216:LYS:HB2	1:A:360:LEU:HD22	2.02	0.41
1:B:132:ARG:O	1:B:133:GLU:CB	2.68	0.41
1:B:241:GLU:HG3	1:C:378:SER:HB3	2.02	0.41
1:C:294:PRO:CB	1:D:381:ARG:CZ	2.99	0.41
1:D:297:ARG:NH2	1:D:329:GLY:O	2.53	0.41
1:E:210:ALA:HB3	1:E:216:LYS:HB3	2.03	0.41
1:F:196:MET:HE1	1:F:425:GLY:N	2.35	0.41
1:A:118:LEU:O	1:A:119:ILE:C	2.63	0.41
1:D:141:ASP:OD2	1:D:297:ARG:HB2	2.21	0.41
1:E:262:ASN:OD1	1:E:268:LEU:HG	2.20	0.41
1:C:233:GLU:CG	1:C:315:GLY:HA3	2.51	0.41
1:D:142:GLU:CA	1:D:328:SER:HB2	2.50	0.41
1:D:381:ARG:C	1:D:383:SER:N	2.77	0.41
1:F:25:PHE:CE1	1:F:67:LEU:HD23	2.56	0.41
1:D:267:LYS:O	1:D:268:LEU:CB	2.68	0.41
1:E:196:MET:HE1	1:E:425:GLY:N	2.35	0.41
1:F:197:THR:HA	1:F:419:GLN:OE1	2.21	0.41
1:E:198:SER:N	1:E:199:GLY:CA	2.77	0.41
1:F:96:VAL:HG22	1:F:97:PRO:HD2	2.03	0.41
1:F:253:CYS:SG	1:F:263:LEU:HD12	2.60	0.41
1:A:104:TYR:CD1	1:B:63:GLU:O	2.73	0.41
1:D:130:TYR:CE1	1:E:119:ILE:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:GLU:N	1:E:134:ASP:CB	2.32	0.41
1:E:293:THR:HA	1:E:294:PRO:HD2	1.79	0.41
1:A:74:LEU:HD22	1:A:83:ILE:HD11	2.03	0.41
1:A:233:GLU:HG3	1:A:315:GLY:HA3	2.02	0.41
1:A:233:GLU:HG2	1:A:315:GLY:HA3	2.03	0.41
1:A:280:MET:O	1:A:281:GLY:C	2.62	0.41
1:A:321:TYR:H	1:A:360:LEU:HB2	1.86	0.41
1:B:267:LYS:O	1:B:268:LEU:CB	2.68	0.41
1:C:209:ALA:HA	1:C:361:SER:O	2.21	0.41
1:C:416:ILE:O	1:C:424:VAL:HG13	2.21	0.41
1:E:197:THR:HA	1:E:419:GLN:OE1	2.21	0.41
1:F:53:HIS:HE1	1:F:57:ARG:HH11	1.68	0.41
1:F:414:ILE:HD11	1:F:429:LEU:HD12	2.02	0.41
1:A:207:ILE:HD12	1:A:390:ALA:CB	2.37	0.41
1:A:208:VAL:HB	1:A:360:LEU:HD23	2.03	0.41
1:A:262:ASN:O	1:A:266:GLY:HA2	2.21	0.41
1:A:364:SER:C	1:A:366:SER:H	2.29	0.41
1:C:48:HIS:O	1:C:49:GLN:C	2.63	0.41
1:E:46:ALA:O	1:E:50:LYS:HD3	2.21	0.41
1:E:104:TYR:HA	1:E:106:ALA:H	1.86	0.41
1:F:83:ILE:HB	1:F:84:GLY:H	1.62	0.41
1:F:148:MET:CE	1:F:148:MET:HA	2.50	0.41
1:F:222:ASN:N	1:F:222:ASN:HD22	2.18	0.41
1:A:42:ASP:HA	1:A:113:SER:OG	2.21	0.40
1:A:74:LEU:HD13	1:A:83:ILE:CD1	2.51	0.40
1:B:47:ALA:HB1	1:B:83:ILE:HG23	2.03	0.40
1:B:48:HIS:CD2	1:B:48:HIS:H	2.39	0.40
1:B:102:VAL:O	1:B:106:ALA:N	2.51	0.40
1:D:65:VAL:HA	1:D:69:THR:HG21	2.03	0.40
1:F:192:GLU:HB3	1:F:427:VAL:HG13	2.04	0.40
1:A:39:ILE:O	1:A:40:PRO:C	2.64	0.40
1:A:53:HIS:HE1	1:A:57:ARG:NH1	2.19	0.40
1:A:83:ILE:HB	1:A:84:GLY:H	1.73	0.40
1:A:217:THR:O	1:A:221:LEU:HG	2.20	0.40
1:B:67:LEU:O	1:B:71:THR:CG2	2.66	0.40
1:F:231:THR:HG23	1:F:233:GLU:H	1.86	0.40
1:A:28:PRO:C	1:A:30:ALA:N	2.79	0.40
1:A:135:GLU:HB3	1:A:138:VAL:HB	2.04	0.40
1:B:207:ILE:HD13	1:B:386:ILE:CG2	2.46	0.40
1:D:145:ARG:HH12	1:D:329:GLY:H	1.69	0.40
1:D:211:ARG:NH1	1:D:368:GLU:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:LEU:HD21	1:E:109:VAL:HB	2.03	0.40
1:A:24:VAL:HG11	1:A:55:MET:SD	2.62	0.40
1:A:261:GLN:HA	1:A:264:ARG:HD2	2.04	0.40
1:B:240:LEU:HD21	1:B:296:ILE:HG13	2.04	0.40
1:D:71:THR:HG22	1:D:89:LEU:CD1	2.52	0.40
1:A:175:MET:HE3	1:A:423:PRO:HA	2.04	0.40
1:C:294:PRO:CB	1:D:381:ARG:HG2	2.52	0.40
1:E:320:ASP:HA	1:E:360:LEU:HD12	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ASN:ND2	1:F:97:PRO:CB[1_565]	2.12	0.08
1:C:178:ASN:CG	1:F:97:PRO:CB[1_565]	2.13	0.07

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	395/454 (87%)	334 (85%)	43 (11%)	18 (5%)	2	18
1	B	366/454 (81%)	308 (84%)	46 (13%)	12 (3%)	3	25
1	C	389/454 (86%)	327 (84%)	37 (10%)	25 (6%)	1	14
1	D	366/454 (81%)	308 (84%)	42 (12%)	16 (4%)	2	19
1	E	380/454 (84%)	325 (86%)	38 (10%)	17 (4%)	2	18
1	F	380/454 (84%)	331 (87%)	33 (9%)	16 (4%)	2	20
All	All	2276/2724 (84%)	1933 (85%)	239 (10%)	104 (5%)	2	18

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	134	ASP
1	A	162	ILE
1	A	179	ARG
1	A	180	ASP
1	A	266	GLY
1	A	268	LEU
1	A	321	TYR
1	B	83	ILE
1	B	104	TYR
1	B	133	GLU
1	B	268	LEU
1	B	321	TYR
1	C	63	GLU
1	C	104	TYR
1	C	133	GLU
1	C	134	ASP
1	C	179	ARG
1	C	180	ASP
1	C	266	GLY
1	C	268	LEU
1	C	321	TYR
1	D	63	GLU
1	D	64	PRO
1	D	83	ILE
1	D	102	VAL
1	D	104	TYR
1	D	134	ASP
1	D	268	LEU
1	D	321	TYR
1	E	63	GLU
1	E	83	ILE
1	E	102	VAL
1	E	134	ASP
1	E	266	GLY
1	E	268	LEU
1	E	321	TYR
1	F	63	GLU
1	F	64	PRO
1	F	102	VAL
1	F	104	TYR
1	F	134	ASP
1	F	266	GLY

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Mol	Chain	Res	Type
1	F	268	LEU
1	F	321	TYR
1	A	163	LYS
1	A	169	THR
1	A	198	SER
1	B	63	GLU
1	B	134	ASP
1	B	136	ILE
1	B	266	GLY
1	C	44	TYR
1	C	101	ASN
1	C	145	ARG
1	C	175	MET
1	D	133	GLU
1	D	136	ILE
1	D	198	SER
1	D	266	GLY
1	A	133	GLU
1	A	267	LYS
1	C	116	ARG
1	C	440	ASN
1	D	78	GLU
1	E	11	PRO
1	E	133	GLU
1	E	198	SER
1	F	78	GLU
1	F	97	PRO
1	F	198	SER
1	A	64	PRO
1	B	64	PRO
1	B	101	ASN
1	B	267	LYS
1	C	64	PRO
1	C	78	GLU
1	C	95	ALA
1	C	181	GLY
1	D	40	PRO
1	D	267	LYS
1	E	49	GLN
1	E	97	PRO
1	E	104	TYR
1	E	267	LYS

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Mol	Chain	Res	Type
1	A	365	ARG
1	C	27	ASP
1	C	83	ILE
1	C	105	TYR
1	C	267	LYS
1	E	29	ALA
1	E	101	ASN
1	F	133	GLU
1	F	267	LYS
1	A	83	ILE
1	A	136	ILE
1	D	142	GLU
1	E	64	PRO
1	A	181	GLY
1	C	102	VAL
1	C	136	ILE
1	F	40	PRO
1	F	83	ILE
1	F	136	ILE

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	341/386 (88%)	309 (91%)	32 (9%)	8	32
1	B	314/386 (81%)	288 (92%)	26 (8%)	10	35
1	C	336/386 (87%)	314 (94%)	22 (6%)	15	43
1	D	314/386 (81%)	289 (92%)	25 (8%)	11	37
1	E	330/386 (86%)	308 (93%)	22 (7%)	15	42
1	F	330/386 (86%)	303 (92%)	27 (8%)	10	36
All	All	1965/2316 (85%)	1811 (92%)	154 (8%)	11	37

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

Mol	Chain	Res	Type
1	A	56	LEU
1	A	60	ASP
1	A	61	ARG
1	A	67	LEU
1	A	80	LEU
1	A	81	GLU
1	A	96	VAL
1	A	115	LEU
1	A	135	GLU
1	A	136	ILE
1	A	161	ASN
1	A	162	ILE
1	A	163	LYS
1	A	164	ASP
1	A	168	GLN
1	A	268	LEU
1	A	271	GLU
1	A	272	ASP
1	A	278	MET
1	A	297	ARG
1	A	306	ARG
1	A	316	MET
1	A	323	GLN
1	A	339	VAL
1	A	340	SER
1	A	362	GLN
1	A	386	ILE
1	A	388	GLN
1	A	391	ASP
1	A	392	ILE
1	A	412	ILE
1	A	439	VAL
1	B	12	GLN
1	B	50	LYS
1	B	56	LEU
1	B	68	VAL
1	B	71	THR
1	B	80	LEU
1	B	81	GLU
1	B	128	ASP
1	B	135	GLU
1	B	136	ILE
1	B	144	ASP

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Mol	Chain	Res	Type
1	B	147	ILE
1	B	148	MET
1	B	186	ILE
1	B	207	ILE
1	B	233	GLU
1	B	269	THR
1	B	271	GLU
1	B	296	ILE
1	B	306	ARG
1	B	316	MET
1	B	321	TYR
1	B	355	VAL
1	B	386	ILE
1	B	388	GLN
1	B	412	ILE
1	C	26	LEU
1	C	50	LYS
1	C	65	VAL
1	C	81	GLU
1	C	115	LEU
1	C	139	LEU
1	C	141	ASP
1	C	148	MET
1	C	163	LYS
1	C	173	ILE
1	C	174	GLU
1	C	195	ARG
1	C	231	THR
1	C	233	GLU
1	C	268	LEU
1	C	271	GLU
1	C	316	MET
1	C	355	VAL
1	C	386	ILE
1	C	388	GLN
1	C	391	ASP
1	C	412	ILE
1	D	12	GLN
1	D	14	ILE
1	D	50	LYS
1	D	56	LEU
1	D	61	ARG

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Mol	Chain	Res	Type
1	D	80	LEU
1	D	81	GLU
1	D	86	VAL
1	D	103	GLU
1	D	108	ILE
1	D	128	ASP
1	D	134	ASP
1	D	136	ILE
1	D	139	LEU
1	D	140	LEU
1	D	147	ILE
1	D	148	MET
1	D	207	ILE
1	D	231	THR
1	D	268	LEU
1	D	271	GLU
1	D	316	MET
1	D	386	ILE
1	D	388	GLN
1	D	412	ILE
1	E	12	GLN
1	E	26	LEU
1	E	50	LYS
1	E	60	ASP
1	E	81	GLU
1	E	105	TYR
1	E	114	VAL
1	E	115	LEU
1	E	139	LEU
1	E	140	LEU
1	E	148	MET
1	E	163	LYS
1	E	171	ASP
1	E	174	GLU
1	E	231	THR
1	E	268	LEU
1	E	271	GLU
1	E	316	MET
1	E	355	VAL
1	E	386	ILE
1	E	388	GLN
1	E	412	ILE

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Mol	Chain	Res	Type
1	F	12	GLN
1	F	50	LYS
1	F	61	ARG
1	F	65	VAL
1	F	77	SER
1	F	80	LEU
1	F	86	VAL
1	F	90	SER
1	F	96	VAL
1	F	103	GLU
1	F	104	TYR
1	F	139	LEU
1	F	147	ILE
1	F	148	MET
1	F	163	LYS
1	F	174	GLU
1	F	268	LEU
1	F	271	GLU
1	F	272	ASP
1	F	297	ARG
1	F	316	MET
1	F	345	SER
1	F	355	VAL
1	F	362	GLN
1	F	386	ILE
1	F	391	ASP
1	F	412	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	53	HIS
1	A	79	GLN
1	A	152	GLN
1	A	172	ASN
1	A	177	HIS
1	A	225	GLN
1	A	226	ASN
1	A	245	GLN
1	A	246	GLN
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	388	GLN
1	A	436	ASN
1	B	12	GLN
1	B	53	HIS
1	B	79	GLN
1	B	225	GLN
1	B	226	ASN
1	B	323	GLN
1	B	388	GLN
1	C	12	GLN
1	C	53	HIS
1	C	79	GLN
1	C	172	ASN
1	C	177	HIS
1	C	225	GLN
1	C	323	GLN
1	C	388	GLN
1	D	49	GLN
1	D	53	HIS
1	D	79	GLN
1	D	225	GLN
1	D	226	ASN
1	D	323	GLN
1	D	388	GLN
1	E	53	HIS
1	E	225	GLN
1	E	226	ASN
1	E	245	GLN
1	E	261	GLN
1	E	388	GLN
1	F	12	GLN
1	F	53	HIS
1	F	225	GLN
1	F	323	GLN
1	F	388	GLN

5.3.3 RNA ⓘ

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	405/454 (89%)	0.40	18 (4%) 39 25	153, 178, 179, 207	0
1	B	376/454 (82%)	0.27	8 (2%) 63 40	175, 178, 179, 186	0
1	C	399/454 (87%)	0.26	12 (3%) 52 32	145, 178, 179, 209	0
1	D	376/454 (82%)	0.25	18 (4%) 35 23	165, 178, 179, 184	0
1	E	392/454 (86%)	0.21	15 (3%) 44 28	169, 178, 179, 198	0
1	F	392/454 (86%)	0.21	7 (1%) 67 42	176, 178, 180, 189	0
All	All	2340/2724 (85%)	0.27	78 (3%) 49 31	145, 178, 179, 209	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	VAL	6.1
1	A	265	THR	4.9
1	F	133	GLU	4.7
1	C	179	ARG	4.6
1	C	178	ASN	4.5
1	D	273	TRP	4.4
1	C	276	LEU	4.2
1	C	195	ARG	3.9
1	D	278	MET	3.8
1	C	126	ALA	3.8
1	C	97	PRO	3.7
1	A	280	MET	3.6
1	A	276	LEU	3.6
1	E	256	GLY	3.6
1	D	328	SER	3.5
1	B	382	GLU	3.4
1	E	346	LEU	3.4
1	D	133	GLU	3.4
1	F	384	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	382	GLU	3.3
1	B	133	GLU	3.3
1	D	140	LEU	3.2
1	E	186	ILE	3.2
1	F	200	PHE	3.2
1	C	104	TYR	3.2
1	F	160	LYS	3.2
1	A	195	ARG	3.1
1	A	305	CYS	3.1
1	D	114	VAL	3.0
1	E	236	ALA	3.0
1	A	273	TRP	3.0
1	E	174	GLU	3.0
1	E	182	GLU	3.0
1	B	273	TRP	2.9
1	A	99	ALA	2.8
1	C	180	ASP	2.7
1	D	430	ALA	2.7
1	D	381	ARG	2.6
1	A	93	ALA	2.6
1	A	15	GLU	2.6
1	F	266	GLY	2.6
1	E	104	TYR	2.5
1	D	250	ARG	2.5
1	C	98	THR	2.5
1	D	427	VAL	2.5
1	A	151	SER	2.4
1	B	233	GLU	2.4
1	E	191	THR	2.4
1	E	194	ASP	2.3
1	E	395	PHE	2.3
1	E	129	GLY	2.3
1	A	179	ARG	2.3
1	B	428	GLN	2.3
1	A	382	GLU	2.3
1	A	327	GLY	2.3
1	D	300	ASP	2.3
1	E	349	LEU	2.3
1	D	149	GLU	2.3
1	D	196	MET	2.2
1	A	272	ASP	2.2
1	C	133	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	272	ASP	2.2
1	D	31	LEU	2.2
1	E	102	VAL	2.1
1	A	271	GLU	2.1
1	B	126	ALA	2.1
1	C	213	SER	2.1
1	F	119	ILE	2.1
1	E	225	GLN	2.1
1	A	252	LEU	2.1
1	A	353	LEU	2.1
1	B	314	LEU	2.1
1	D	211	ARG	2.0
1	E	251	MET	2.0
1	A	264	ARG	2.0
1	B	375	PRO	2.0
1	D	98	THR	2.0
1	D	263	LEU	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.