



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:28 PM UTC

PDB ID : 1UIJ / pdb_00001uij
Title : Crystal Structure Of Soybean beta-Conglycinin Beta Homotrimer (I122M/K124W)
Authors : Maruyama, N.; Maruyama, Y.; Tsuruki, T.; Okuda, E.; Yoshikawa, M.; Utsumi, S.
Deposited on : 2003-07-16
Resolution : 2.50 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

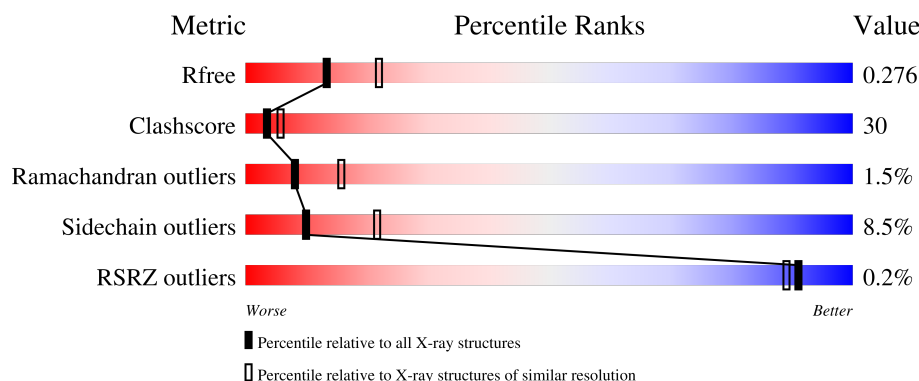
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	416	 49% 37% 5% 9%
1	B	416	 46% 37% 6% 11%
1	C	416	 39% 38% 5% 17%
1	D	416	 48% 37% 6% 9%
1	E	416	 45% 40% • 11%

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Mol	Chain	Length	Quality of chain
1	F	416	36% 42% 6% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18133 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 subunit of beta conglycinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3087	1947	550	589	1			
1	B	370	Total	C	N	O	S	0	0	0
			3022	1911	538	572	1			
1	C	346	Total	C	N	O	S	0	0	0
			2824	1797	494	532	1			
1	D	377	Total	C	N	O	S	0	0	0
			3087	1947	550	589	1			
1	E	370	Total	C	N	O	S	0	0	0
			3022	1911	538	572	1			
1	F	346	Total	C	N	O	S	0	0	0
			2824	1797	494	532	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	MET	ILE	engineered mutation	UNP P25974
A	124	TRP	LYS	engineered mutation	UNP P25974
B	122	MET	ILE	engineered mutation	UNP P25974
B	124	TRP	LYS	engineered mutation	UNP P25974
C	122	MET	ILE	engineered mutation	UNP P25974
C	124	TRP	LYS	engineered mutation	UNP P25974
D	122	MET	ILE	engineered mutation	UNP P25974
D	124	TRP	LYS	engineered mutation	UNP P25974
E	122	MET	ILE	engineered mutation	UNP P25974
E	124	TRP	LYS	engineered mutation	UNP P25974
F	122	MET	ILE	engineered mutation	UNP P25974
F	124	TRP	LYS	engineered mutation	UNP P25974

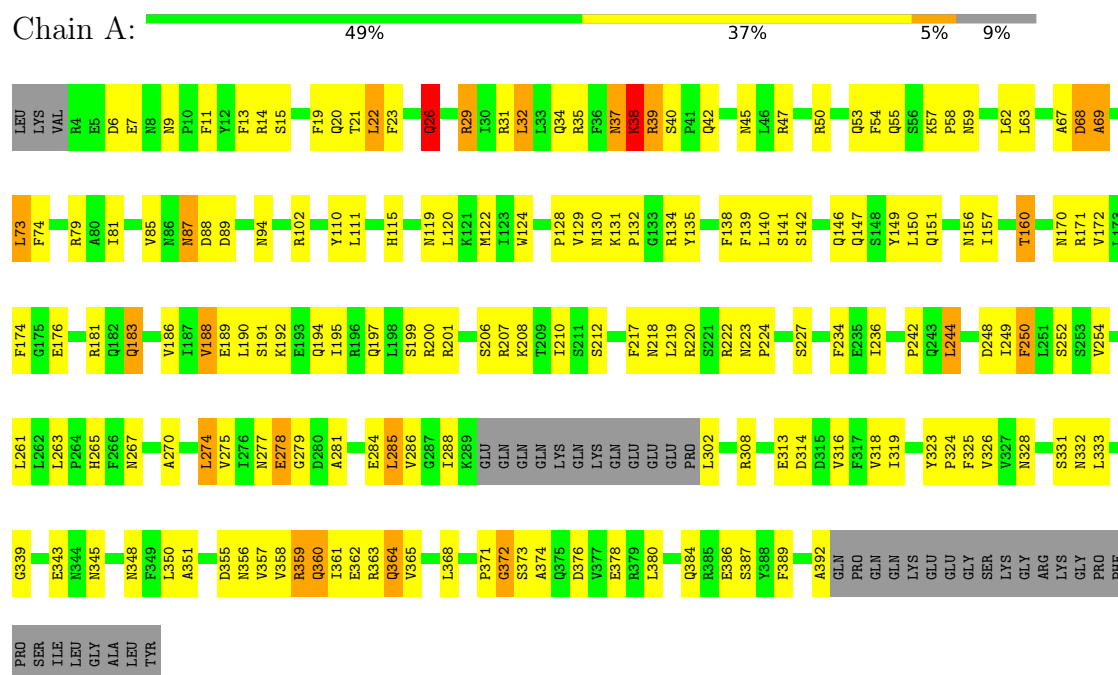
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	62	Total 62	O 62	0	0
2	B	53	Total 53	O 53	0	0
2	C	19	Total 19	O 19	0	0
2	D	65	Total 65	O 65	0	0
2	E	47	Total 47	O 47	0	0
2	F	21	Total 21	O 21	0	0

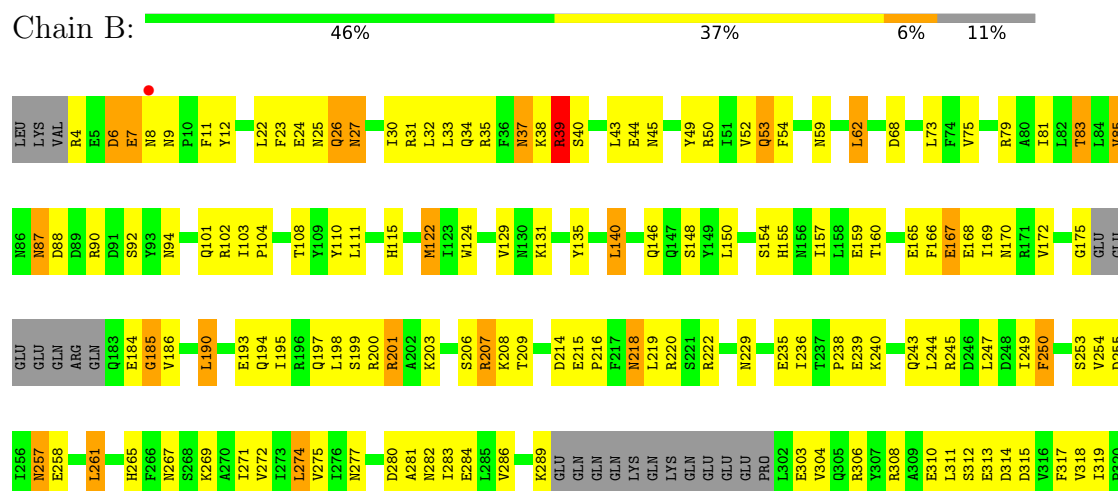
3 Residue-property plots

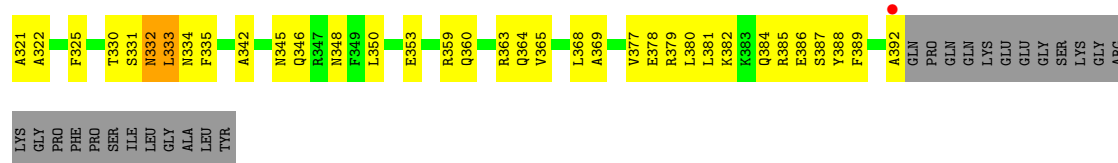
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

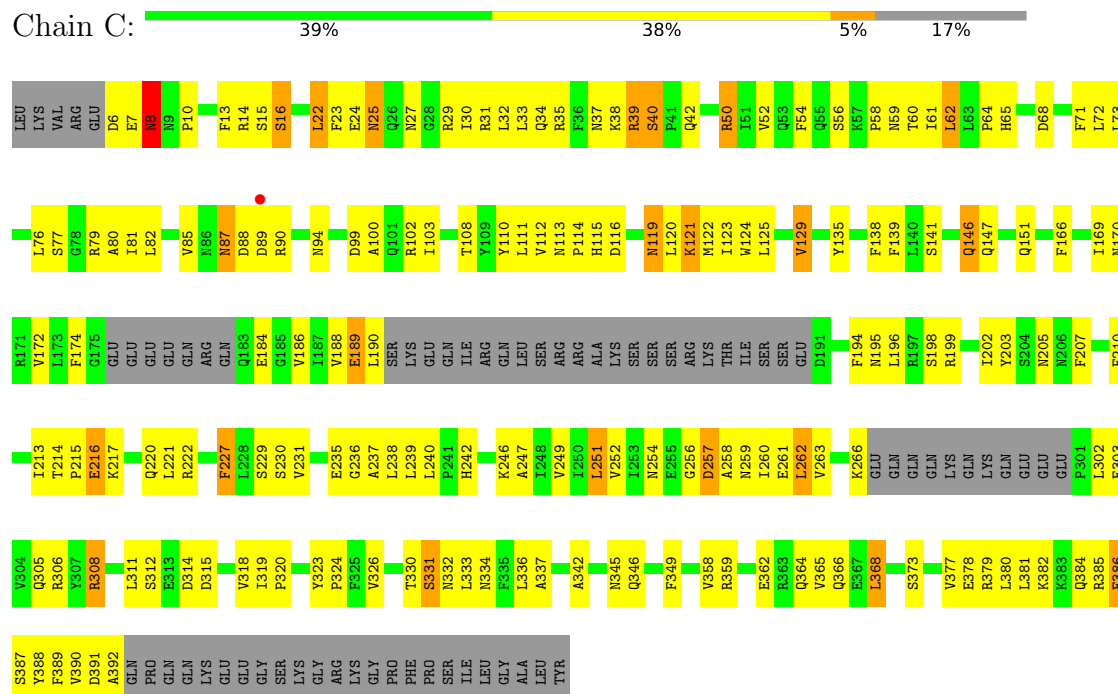


- Molecule 1: beta subunit of beta conglycinin

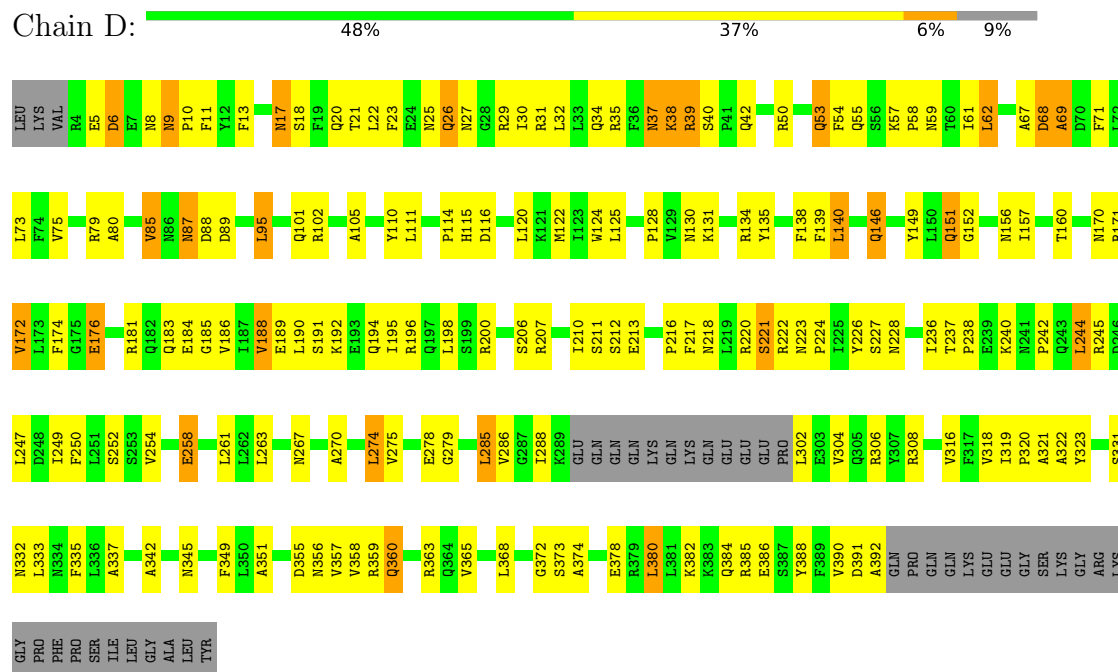


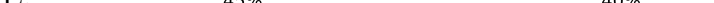


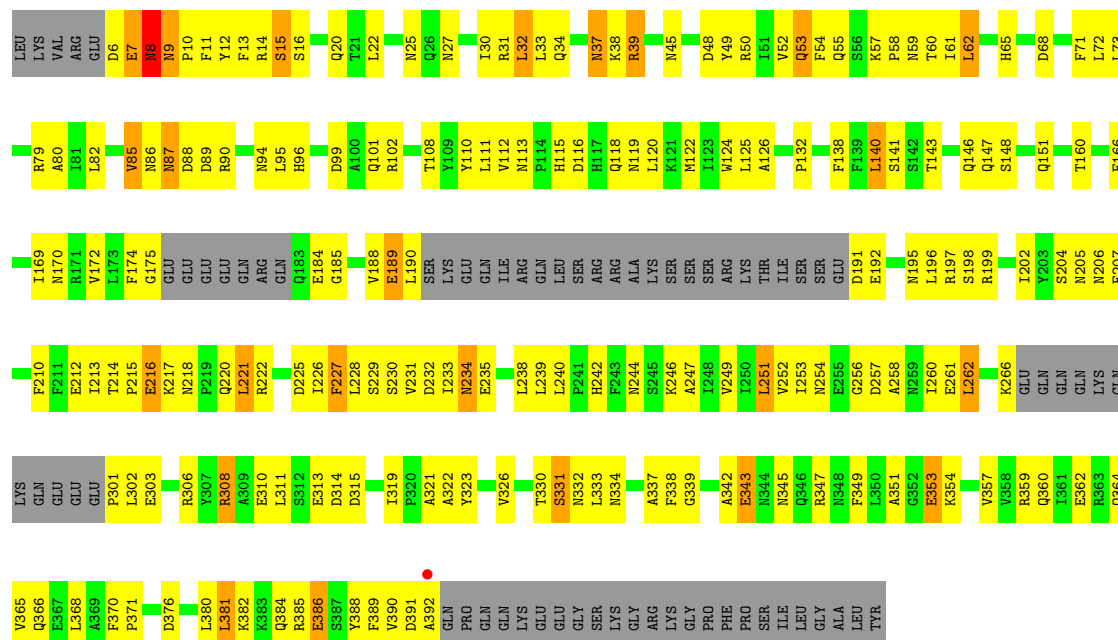
- Molecule 1: beta subunit of beta conglycinin



- Molecule 1: beta subunit of beta conglycinin



- Chain E:  45% 40% • 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.26Å 62.58Å 159.01Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 90.9 (8.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.273 0.225 , 0.276	Depositor DCC
R_{free} test set	4277 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 79.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18133	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.46	0/3150	0.97	11/4260 (0.3%)
1	B	0.46	1/3084 (0.0%)	0.97	9/4171 (0.2%)
1	C	0.38	0/2886	0.91	5/3910 (0.1%)
1	D	0.46	0/3150	0.98	8/4260 (0.2%)
1	E	0.45	0/3084	0.96	7/4171 (0.2%)
1	F	0.39	0/2886	0.90	8/3910 (0.2%)
All	All	0.44	1/18240 (0.0%)	0.95	48/24682 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	MET	SD-CE	-5.59	1.65	1.79

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	ALA	N-CA-C	8.79	123.30	112.23
1	D	26	GLN	N-CA-C	-8.41	103.02	113.28
1	D	172	VAL	N-CA-C	8.23	118.80	110.82
1	D	342	ALA	N-CA-C	7.61	120.64	111.82
1	A	38	LYS	N-CA-C	-7.29	103.33	111.28
1	C	129	VAL	N-CA-C	7.14	117.95	111.81
1	A	26	GLN	N-CA-C	-7.12	104.59	113.28
1	F	342	ALA	N-CA-C	7.04	121.14	112.54
1	B	342	ALA	N-CA-C	6.88	119.80	111.82
1	E	342	ALA	N-CA-C	6.39	120.28	112.23
1	D	62	LEU	N-CA-C	-6.37	99.50	109.25
1	A	172	VAL	N-CA-C	6.35	117.13	110.72
1	B	39	ARG	N-CA-C	-6.30	103.11	111.24
1	B	129	VAL	N-CA-C	6.26	118.21	111.58
1	F	172	VAL	N-CA-C	6.11	117.66	111.00
1	A	129	VAL	N-CA-C	6.02	116.99	111.81
1	E	272	VAL	N-CA-C	6.02	117.25	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ASN	N-CA-C	-5.99	105.62	113.17
1	D	360	GLN	N-CA-C	-5.98	105.95	113.72
1	C	249	VAL	N-CA-C	5.96	117.59	108.71
1	D	69	ALA	N-CA-C	5.91	117.22	108.60
1	F	249	VAL	N-CA-C	5.89	116.78	108.36
1	E	253	SER	N-CA-C	-5.74	99.54	108.90
1	D	247	LEU	N-CA-C	-5.74	106.32	113.38
1	A	20	GLN	N-CA-C	-5.69	99.96	109.24
1	F	354	LYS	N-CA-C	5.62	118.00	110.35
1	B	271	ILE	N-CA-C	-5.57	99.86	107.99
1	F	189	GLU	N-CA-C	5.54	119.67	113.02
1	B	62	LEU	N-CA-C	-5.51	100.19	108.96
1	B	272	VAL	N-CA-C	5.51	116.24	108.36
1	E	166	PHE	N-CA-C	5.46	117.23	111.28
1	B	333	LEU	N-CA-C	5.41	118.38	109.72
1	A	63	LEU	N-CA-C	5.34	117.76	110.01
1	C	8	ASN	N-CA-C	-5.21	104.91	113.50
1	A	183	GLN	N-CA-C	-5.17	103.57	110.55
1	B	27	ASN	N-CA-C	5.16	118.73	112.23
1	F	62	LEU	N-CA-C	-5.16	100.76	108.96
1	A	208	LYS	N-CA-C	5.13	118.64	112.38
1	A	19	PHE	N-CA-C	5.10	117.21	108.90
1	C	119	ASN	N-CA-C	5.09	117.75	109.86
1	F	8	ASN	N-CA-C	-5.09	105.10	113.50
1	E	109	TYR	N-CA-C	5.08	115.86	108.14
1	F	204	SER	N-CA-C	5.07	116.32	107.49
1	D	333	LEU	N-CA-C	5.05	117.81	109.72
1	E	196	ARG	N-CA-C	-5.05	105.96	111.82
1	E	8	ASN	N-CA-C	-5.04	106.72	112.92
1	A	69	ALA	N-CA-C	5.03	116.71	109.07
1	A	15	SER	N-CA-C	5.02	117.48	111.71

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	3087	0	3004	163	0
1	B	3022	0	2950	160	0
1	C	2824	0	2739	206	0
1	D	3087	0	3004	170	0
1	E	3022	0	2950	183	0
1	F	2824	0	2739	216	0
2	A	62	0	0	3	0
2	B	53	0	0	3	0
2	C	19	0	0	0	0
2	D	65	0	0	4	0
2	E	47	0	0	5	0
2	F	21	0	0	3	0
All	All	18133	0	17386	1043	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 30.

All (1043) 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:F:111:LEU:HD21	1:F:122:MET:HE1	1.28	1.10
1:B:59:ASN:HD22	1:B:195:ILE:HD12	1.03	1.07
1:E:90:ARG:HH11	1:F:362:GLU:HG2	1.19	1.05
1:E:59:ASN:HD22	1:E:195:ILE:HD12	1.20	1.05
1:B:111:LEU:HD21	1:B:122:MET:HE1	1.06	1.03
1:A:26:GLN:H	1:A:26:GLN:HE21	1.04	1.03
1:A:183:GLN:HG2	1:A:188:VAL:HG11	1.42	1.01
1:D:111:LEU:HD21	1:D:122:MET:HE1	1.40	1.01
1:B:26:GLN:H	1:B:26:GLN:NE2	1.61	0.99
1:E:37:ASN:HD22	1:E:37:ASN:H	1.11	0.98
1:E:90:ARG:NH1	1:F:362:GLU:HG2	1.79	0.98
1:A:111:LEU:HD21	1:A:122:MET:HE1	1.45	0.97
1:D:183:GLN:HG2	1:D:188:VAL:HG11	1.45	0.96
1:E:79:ARG:HD2	1:E:94:ASN:HD21	1.29	0.96
1:A:348:ASN:HD22	1:A:357:VAL:HB	1.29	0.95
1:E:111:LEU:HD21	1:E:122:MET:HE1	1.49	0.94
1:C:384:GLN:HE21	1:C:386:GLU:H	1.08	0.94
1:C:384:GLN:NE2	1:C:386:GLU:HB2	1.83	0.93
1:E:122:MET:HE3	1:E:124:TRP:HE1	1.34	0.93
1:B:59:ASN:HD22	1:B:195:ILE:CD1	1.82	0.91
1:A:261:LEU:HD22	1:A:392:ALA:HB2	1.52	0.91
1:B:261:LEU:HD22	1:B:392:ALA:HB2	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASN:ND2	1:B:195:ILE:HD12	1.86	0.90
1:C:50:ARG:HH21	1:C:50:ARG:HB3	1.35	0.90
1:A:37:ASN:HD22	1:A:37:ASN:H	1.20	0.90
1:B:79:ARG:NH1	1:B:94:ASN:HD21	1.71	0.88
1:A:120:LEU:HD21	1:A:122:MET:HE2	1.54	0.88
1:A:364:GLN:NE2	1:A:364:GLN:H	1.71	0.88
1:D:29:ARG:HD3	1:D:31:ARG:HG3	1.56	0.87
1:B:26:GLN:H	1:B:26:GLN:HE21	1.22	0.87
1:F:79:ARG:HE	1:F:94:ASN:HD21	1.20	0.86
1:B:111:LEU:CD2	1:B:122:MET:HE1	2.00	0.86
1:B:37:ASN:H	1:B:37:ASN:HD22	1.19	0.86
1:E:218:ASN:HD22	1:E:220:ARG:H	1.23	0.86
1:D:122:MET:HE3	1:D:124:TRP:HE1	1.40	0.85
1:A:35:ARG:NH1	1:A:134:ARG:HD2	1.92	0.84
1:B:111:LEU:HD21	1:B:122:MET:CE	2.00	0.84
1:C:170:ASN:HD22	1:C:174:PHE:HB2	1.43	0.83
1:A:371:PRO:HG3	1:C:174:PHE:O	1.78	0.83
1:E:111:LEU:HD21	1:E:122:MET:CE	2.08	0.82
1:C:13:PHE:CE1	1:C:39:ARG:HG3	2.14	0.82
1:F:14:ARG:HG2	1:F:16:SER:HB3	1.61	0.82
1:D:111:LEU:HD21	1:D:122:MET:CE	2.10	0.82
1:F:34:GLN:NE2	1:F:39:ARG:HG2	1.93	0.82
1:C:32:LEU:HD23	1:C:52:VAL:HG22	1.60	0.82
1:F:302:LEU:HD22	1:F:302:LEU:H	1.43	0.81
1:A:218:ASN:ND2	1:A:220:ARG:H	1.77	0.81
1:D:218:ASN:HD22	1:D:220:ARG:H	1.26	0.81
1:E:207:ARG:HH11	1:E:207:ARG:HB3	1.44	0.81
1:D:176:GLU:HB2	2:D:437:HOH:O	1.79	0.81
1:A:26:GLN:H	1:A:26:GLN:NE2	1.78	0.81
1:A:26:GLN:HE21	1:A:26:GLN:N	1.78	0.81
1:D:34:GLN:OE1	1:D:39:ARG:HD2	1.80	0.80
1:C:386:GLU:HB3	1:C:390:VAL:HG12	1.62	0.80
1:A:156:ASN:O	1:A:160:THR:HG22	1.80	0.80
1:B:79:ARG:HH11	1:B:94:ASN:HD21	1.24	0.80
1:C:170:ASN:ND2	1:C:174:PHE:HB2	1.95	0.79
1:B:219:LEU:HD13	1:B:236:ILE:HG12	1.65	0.79
1:C:79:ARG:HD2	1:C:94:ASN:HD21	1.48	0.78
1:E:26:GLN:NE2	1:E:26:GLN:H	1.82	0.78
1:D:17:ASN:HD22	1:D:17:ASN:C	1.91	0.77
1:C:214:THR:H	1:C:217:LYS:HE3	1.49	0.77
1:A:218:ASN:HD22	1:A:220:ARG:H	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASP:HA	1:C:87:ASN:O	1.84	0.77
1:A:189:GLU:O	1:A:190:LEU:HD12	1.84	0.76
1:E:59:ASN:HA	1:E:195:ILE:HD11	1.66	0.76
1:B:44:GLU:HG3	2:B:435:HOH:O	1.84	0.76
1:F:52:VAL:HB	1:F:124:TRP:HB2	1.67	0.76
1:D:261:LEU:HD21	1:D:390:VAL:HG22	1.68	0.75
1:A:29:ARG:HD3	1:A:31:ARG:HG3	1.67	0.75
1:D:261:LEU:HD21	1:D:390:VAL:CG2	2.16	0.75
1:C:236:GLY:O	1:C:392:ALA:HB3	1.87	0.75
1:A:384:GLN:HE21	1:A:386:GLU:H	1.33	0.75
1:F:196:LEU:HD13	1:F:213:ILE:HG12	1.67	0.75
1:A:261:LEU:HB3	1:A:328:ASN:HD22	1.52	0.75
1:E:37:ASN:HD22	1:E:37:ASN:N	1.85	0.75
1:C:35:ARG:HG2	1:C:50:ARG:HE	1.51	0.75
1:B:81:ILE:CD1	1:B:199:SER:HB3	2.17	0.74
1:D:218:ASN:ND2	1:D:220:ARG:H	1.85	0.74
1:F:15:SER:HB3	1:F:314:ASP:O	1.87	0.74
1:A:38:LYS:HD3	1:A:39:ARG:N	2.02	0.74
1:D:191:SER:OG	1:D:194:GLN:HG3	1.86	0.74
1:B:32:LEU:HD11	1:B:50:ARG:CZ	2.16	0.74
1:A:111:LEU:HD21	1:A:122:MET:CE	2.16	0.74
1:E:277:ASN:HB3	1:E:334:ASN:HD22	1.52	0.74
1:C:6:ASP:O	1:C:8:ASN:N	2.20	0.74
1:A:81:ILE:HD13	1:A:199:SER:HA	1.68	0.74
1:B:382:LYS:HZ3	1:B:385:ARG:HH12	1.34	0.74
1:A:380:LEU:HD11	1:C:169:ILE:HA	1.69	0.73
1:F:31:ARG:HE	1:F:53:GLN:HE21	1.33	0.73
1:C:306:ARG:HD3	1:C:308:ARG:NH1	2.02	0.73
1:E:111:LEU:CD2	1:E:122:MET:HE1	2.19	0.73
1:E:59:ASN:HA	1:E:195:ILE:CD1	2.17	0.73
1:C:199:ARG:HD3	1:C:213:ILE:CD1	2.19	0.73
1:F:13:PHE:CE1	1:F:39:ARG:HG3	2.24	0.72
1:B:140:LEU:HD11	1:C:358:VAL:HG22	1.71	0.72
1:C:30:ILE:HG12	1:C:54:PHE:HD1	1.54	0.72
1:C:214:THR:H	1:C:217:LYS:CE	2.02	0.72
1:A:356:ASN:HB3	1:A:359:ARG:HG2	1.72	0.71
1:D:207:ARG:HH11	1:D:207:ARG:HG3	1.55	0.71
1:F:384:GLN:HE21	1:F:386:GLU:H	1.37	0.71
1:E:110:TYR:OH	1:F:362:GLU:HG3	1.90	0.71
1:E:169:ILE:HA	1:F:380:LEU:HD11	1.73	0.71
1:C:306:ARG:HD3	1:C:308:ARG:HH12	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ASN:C	1:D:9:ASN:HD22	1.99	0.71
1:E:363:ARG:HG2	1:E:378:GLU:OE1	1.90	0.70
1:D:363:ARG:HG2	1:D:374:ALA:HB1	1.72	0.70
1:B:363:ARG:HG2	1:B:378:GLU:OE1	1.91	0.70
1:E:218:ASN:ND2	1:E:220:ARG:H	1.90	0.70
1:A:261:LEU:HB3	1:A:328:ASN:ND2	2.05	0.70
1:E:102:ARG:HB3	1:E:243:GLN:HE21	1.57	0.70
1:F:111:LEU:HD21	1:F:122:MET:CE	2.14	0.69
1:B:257:ASN:HD22	1:B:257:ASN:N	1.89	0.69
1:E:59:ASN:ND2	1:E:195:ILE:HD12	2.01	0.69
1:C:102:ARG:H	1:C:220:GLN:NE2	1.90	0.69
1:B:39:ARG:HG3	1:B:40:SER:N	2.07	0.69
1:D:306:ARG:HD2	1:D:308:ARG:NH2	2.07	0.69
1:D:384:GLN:HE21	1:D:386:GLU:H	1.39	0.69
1:A:59:ASN:HA	1:A:195:ILE:HD11	1.74	0.69
1:A:68:ASP:HB3	1:A:135:TYR:HB2	1.75	0.69
1:B:90:ARG:CZ	1:C:362:GLU:HG2	2.22	0.69
1:F:197:ARG:HH22	1:F:232:ASP:CG	2.01	0.69
1:F:205:ASN:HD21	1:F:389:PHE:HB2	1.58	0.69
1:C:35:ARG:CG	1:C:50:ARG:HE	2.06	0.69
1:D:37:ASN:H	1:D:37:ASN:HD22	1.41	0.69
1:F:261:GLU:CD	1:F:308:ARG:HH21	2.01	0.69
1:D:198:LEU:HD21	1:E:364:GLN:HB2	1.75	0.68
1:A:87:ASN:HD22	1:A:88:ASP:N	1.91	0.68
1:C:254:ASN:HB3	1:C:334:ASN:HD22	1.59	0.68
1:F:235:GLU:H	1:F:332:ASN:HD22	1.40	0.68
1:B:219:LEU:CD1	1:B:236:ILE:HG12	2.22	0.68
1:D:258:GLU:HG3	1:D:331:SER:HA	1.76	0.68
1:E:32:LEU:HD11	1:E:50:ARG:CZ	2.23	0.68
1:B:377:VAL:O	1:B:381:LEU:HG	1.92	0.68
1:C:260:ILE:HD12	1:C:311:LEU:HD11	1.76	0.68
1:A:35:ARG:HG3	1:A:50:ARG:NH2	2.09	0.68
1:A:35:ARG:HH12	1:A:134:ARG:HD2	1.59	0.68
1:D:210:ILE:HD11	1:D:236:ILE:HD12	1.76	0.68
1:E:207:ARG:HH11	1:E:207:ARG:CB	2.07	0.68
1:F:233:ILE:HD12	1:F:333:LEU:HD23	1.74	0.67
1:B:160:THR:HG21	1:C:392:ALA:HB2	1.76	0.67
1:D:357:VAL:HG23	1:F:86:ASN:O	1.95	0.67
1:F:364:GLN:CD	1:F:364:GLN:H	2.03	0.67
1:F:221:LEU:HG	1:F:226:ILE:O	1.94	0.67
1:A:368:LEU:HD23	1:C:188:VAL:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ILE:HB	1:E:112:VAL:HG22	1.77	0.67
1:D:59:ASN:HA	1:D:195:ILE:HD11	1.77	0.66
1:E:4:ARG:HB2	1:E:306:ARG:O	1.95	0.66
1:C:13:PHE:HE1	1:C:39:ARG:HG3	1.60	0.66
1:D:85:VAL:HG23	1:E:360:GLN:HB2	1.77	0.66
1:D:111:LEU:CD2	1:D:122:MET:HE1	2.20	0.66
1:F:37:ASN:HD22	1:F:37:ASN:H	1.40	0.66
1:A:69:ALA:HB2	1:A:128:PRO:HA	1.78	0.66
1:D:238:PRO:HB3	1:D:245:ARG:HA	1.78	0.66
1:E:116:ASP:CG	1:E:192:LYS:HE3	2.20	0.66
1:C:39:ARG:HG2	1:C:39:ARG:HH11	1.59	0.66
1:C:14:ARG:HG2	1:C:16:SER:HB3	1.78	0.66
1:D:29:ARG:HD3	1:D:31:ARG:CG	2.26	0.66
1:C:54:PHE:CD2	1:C:122:MET:HE2	2.30	0.65
1:D:183:GLN:CG	1:D:188:VAL:HG11	2.22	0.65
1:E:81:ILE:HD13	1:E:199:SER:HA	1.78	0.65
1:B:155:HIS:O	1:B:159:GLU:HG3	1.96	0.65
1:B:283:ILE:HD12	1:B:311:LEU:HD11	1.78	0.65
1:A:34:GLN:NE2	1:A:38:LYS:HE2	2.12	0.65
1:F:132:PRO:HA	2:F:421:HOH:O	1.95	0.65
1:A:35:ARG:CG	1:A:50:ARG:NH2	2.59	0.65
1:B:37:ASN:HD22	1:B:37:ASN:N	1.90	0.65
1:F:37:ASN:HD22	1:F:37:ASN:N	1.93	0.65
1:F:260:ILE:HD12	1:F:311:LEU:HD11	1.79	0.65
1:A:274:LEU:HD12	1:A:274:LEU:C	2.22	0.65
1:B:284:GLU:HG2	1:B:308:ARG:HG2	1.77	0.65
1:F:234:ASN:N	1:F:234:ASN:HD22	1.95	0.65
1:F:313:GLU:O	1:F:314:ASP:HB2	1.96	0.65
1:C:151:GLN:HG2	1:C:174:PHE:CZ	2.31	0.65
1:C:199:ARG:HD3	1:C:213:ILE:HD11	1.79	0.64
1:C:379:ARG:HG3	1:C:379:ARG:HH11	1.62	0.64
1:D:59:ASN:HD22	1:D:195:ILE:CD1	2.10	0.64
1:D:156:ASN:O	1:D:160:THR:HG22	1.97	0.64
1:E:384:GLN:HE21	1:E:386:GLU:H	1.45	0.64
1:C:239:LEU:O	1:C:326:VAL:HG23	1.97	0.64
1:F:258:ALA:HB2	1:F:333:LEU:HD22	1.80	0.64
1:F:9:ASN:C	1:F:9:ASN:HD22	2.04	0.64
1:B:6:ASP:O	1:B:7:GLU:HB2	1.97	0.64
1:A:34:GLN:CD	1:A:38:LYS:HE2	2.22	0.64
1:A:183:GLN:HG2	1:A:188:VAL:CG1	2.25	0.63
1:C:227:PHE:C	1:C:227:PHE:CD2	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LEU:HD12	1:C:251:LEU:C	2.23	0.63
1:D:358:VAL:HG22	1:F:140:LEU:HD11	1.79	0.63
1:C:373:SER:O	1:C:377:VAL:HG23	1.98	0.63
1:D:35:ARG:HB2	1:D:38:LYS:HB3	1.81	0.63
1:D:237:THR:H	1:D:240:LYS:HE3	1.64	0.63
1:A:183:GLN:CG	1:A:188:VAL:HG11	2.24	0.63
1:C:252:VAL:HG22	1:C:336:LEU:HB3	1.81	0.63
1:F:199:ARG:HH12	1:F:217:LYS:HD2	1.62	0.63
1:C:195:ASN:HB3	1:C:198:SER:HB2	1.80	0.63
1:C:378:GLU:O	1:C:382:LYS:HG3	1.99	0.63
1:C:50:ARG:HH21	1:C:50:ARG:CB	2.11	0.63
1:B:81:ILE:HD13	1:B:199:SER:HB3	1.79	0.63
1:E:168:GLU:O	1:E:172:VAL:HG23	1.99	0.63
1:E:218:ASN:HD21	1:E:220:ARG:HB2	1.63	0.63
1:F:195:ASN:HD22	1:F:198:SER:N	1.96	0.63
1:F:170:ASN:ND2	1:F:174:PHE:HB2	2.13	0.62
1:D:59:ASN:ND2	1:D:195:ILE:HD12	2.14	0.62
1:D:189:GLU:O	1:D:190:LEU:HD23	1.99	0.62
1:B:73:LEU:HG	1:B:124:TRP:CD1	2.35	0.62
1:E:83:THR:HB	1:E:92:SER:OG	2.00	0.62
1:C:214:THR:OG1	1:C:217:LYS:HE2	2.00	0.62
1:D:285:LEU:HD21	1:D:323:TYR:HB3	1.79	0.62
1:B:220:ARG:HH22	1:B:255:ASP:CG	2.08	0.62
1:B:258:GLU:H	1:B:332:ASN:HD22	1.47	0.62
1:B:269:LYS:H	1:B:345:ASN:HD22	1.47	0.61
1:B:277:ASN:HB3	1:B:334:ASN:HD22	1.64	0.61
1:E:87:ASN:HD22	1:E:88:ASP:N	1.97	0.61
1:C:151:GLN:HG2	1:C:174:PHE:CE1	2.35	0.61
1:F:238:LEU:HD22	1:F:392:ALA:HB2	1.81	0.61
1:A:212:SER:O	1:A:242:PRO:HG2	2.00	0.61
1:C:122:MET:HE3	1:C:124:TRP:HE1	1.64	0.61
1:E:206:SER:H	1:E:209:THR:CG2	2.13	0.61
1:B:382:LYS:HE2	1:B:385:ARG:NH2	2.15	0.61
1:D:355:ASP:HA	1:F:87:ASN:O	2.01	0.61
1:C:80:ALA:HB2	1:C:120:LEU:HD13	1.83	0.61
1:D:252:SER:OG	1:D:337:ALA:HB3	2.00	0.61
1:F:235:GLU:H	1:F:332:ASN:ND2	1.97	0.61
1:E:54:PHE:CD2	1:E:122:MET:HE2	2.36	0.61
1:F:306:ARG:HD3	1:F:308:ARG:HH12	1.66	0.61
1:F:39:ARG:HG2	1:F:39:ARG:HH11	1.66	0.61
1:D:261:LEU:HD23	1:D:261:LEU:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:PHE:O	1:D:356:ASN:HA	2.02	0.60
1:A:35:ARG:N	1:A:50:ARG:NH2	2.48	0.60
1:A:263:LEU:HD13	1:A:351:ALA:O	2.00	0.60
1:D:31:ARG:HH21	1:D:53:GLN:NE2	1.98	0.60
1:A:131:LYS:HE2	2:A:442:HOH:O	2.01	0.60
1:C:54:PHE:HD2	1:C:122:MET:HE2	1.65	0.60
1:C:252:VAL:CG2	1:C:336:LEU:HB3	2.32	0.60
1:C:384:GLN:HE21	1:C:386:GLU:N	1.90	0.60
1:E:31:ARG:HH21	1:E:53:GLN:HE22	1.49	0.60
1:E:79:ARG:HD2	1:E:94:ASN:ND2	2.09	0.60
1:C:207:PHE:CE1	1:C:391:ASP:HB2	2.36	0.60
1:A:170:ASN:HD22	1:A:174:PHE:HB2	1.67	0.60
1:B:261:LEU:N	1:B:261:LEU:HD23	2.17	0.60
1:C:89:ASP:CG	1:C:90:ARG:H	2.09	0.60
1:C:312:SER:O	1:C:315:ASP:HB2	2.01	0.60
1:E:122:MET:CE	1:E:124:TRP:HE1	2.12	0.60
1:B:26:GLN:HE21	1:B:26:GLN:N	1.97	0.60
1:B:87:ASN:HD22	1:B:88:ASP:N	1.98	0.60
1:C:262:LEU:HD21	1:C:323:TYR:HB3	1.83	0.60
1:F:240:LEU:HD12	1:F:388:TYR:N	2.16	0.60
1:F:31:ARG:HE	1:F:53:GLN:NE2	1.98	0.60
1:E:9:ASN:HD22	1:E:9:ASN:C	2.09	0.60
1:E:37:ASN:H	1:E:37:ASN:ND2	1.91	0.60
1:E:172:VAL:HG11	1:F:376:ASP:O	2.01	0.60
1:F:359:ARG:HD3	1:F:381:LEU:O	2.02	0.60
1:E:102:ARG:H	1:E:243:GLN:NE2	2.00	0.59
1:F:79:ARG:O	1:F:120:LEU:HD13	2.02	0.59
1:C:246:LYS:H	1:C:345:ASN:ND2	2.01	0.59
1:D:222:ARG:HH21	1:D:222:ARG:HG3	1.67	0.59
1:C:61:ILE:CD1	1:C:112:VAL:HG22	2.33	0.59
1:F:227:PHE:C	1:F:227:PHE:CD2	2.81	0.59
1:F:235:GLU:CD	1:F:331:SER:HA	2.27	0.59
1:B:289:LYS:N	1:B:303:GLU:O	2.34	0.59
1:E:122:MET:HE3	1:E:124:TRP:NE1	2.12	0.59
1:F:170:ASN:HD22	1:F:174:PHE:HB2	1.67	0.59
1:A:37:ASN:HD22	1:A:37:ASN:N	1.92	0.59
1:D:116:ASP:OD1	1:D:192:LYS:HE2	2.03	0.59
1:E:313:GLU:O	1:E:314:ASP:HB2	2.03	0.59
1:C:196:LEU:HD23	1:C:230:SER:HB2	1.85	0.59
1:D:87:ASN:HD22	1:D:88:ASP:N	2.00	0.59
1:F:102:ARG:HB3	1:F:220:GLN:HE21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:HD13	1:C:50:ARG:HH22	1.67	0.58
1:C:263:VAL:CG1	1:C:324:PRO:HB2	2.33	0.58
1:C:61:ILE:HD12	1:C:112:VAL:HG22	1.85	0.58
1:D:68:ASP:HB3	1:D:135:TYR:HB2	1.83	0.58
1:D:218:ASN:HD22	1:D:220:ARG:N	1.99	0.58
1:D:363:ARG:CG	1:D:374:ALA:HB1	2.33	0.58
1:E:353:GLU:OE1	1:E:385:ARG:NH1	2.37	0.58
1:F:244:ASN:HB3	1:F:345:ASN:HD21	1.68	0.58
1:A:191:SER:OG	1:A:194:GLN:HG3	2.03	0.58
1:B:218:ASN:ND2	1:B:220:ARG:H	2.02	0.58
1:C:119:ASN:N	1:C:119:ASN:HD22	2.02	0.58
1:F:57:LYS:HB3	1:F:58:PRO:HD2	1.86	0.58
1:F:111:LEU:CD2	1:F:122:MET:HE1	2.20	0.58
1:B:35:ARG:HD2	1:B:38:LYS:HD2	1.85	0.58
1:A:210:ILE:HD11	1:A:236:ILE:HD12	1.86	0.58
1:B:200:ARG:HG3	1:B:201:ARG:HG3	1.85	0.58
1:F:330:THR:O	1:F:331:SER:HB3	2.03	0.58
1:F:253:ILE:HD11	1:F:311:LEU:HD12	1.84	0.58
1:D:35:ARG:NH1	1:D:134:ARG:HD2	2.19	0.58
1:D:288:ILE:HG21	1:D:302:LEU:HD13	1.85	0.58
1:B:33:LEU:O	1:B:50:ARG:NH2	2.37	0.57
1:C:14:ARG:HA	1:C:315:ASP:OD2	2.05	0.57
1:C:27:ASN:HB3	1:C:60:THR:HG21	1.84	0.57
1:C:102:ARG:N	1:C:220:GLN:NE2	2.52	0.57
1:F:6:ASP:O	1:F:8:ASN:N	2.37	0.57
1:F:30:ILE:HG12	1:F:54:PHE:HD1	1.68	0.57
1:C:256:GLY:HA3	1:C:332:ASN:O	2.05	0.57
1:F:199:ARG:HH22	1:F:217:LYS:HD2	1.69	0.57
1:A:138:PHE:HB3	1:A:149:TYR:CD2	2.39	0.57
1:E:277:ASN:CB	1:E:334:ASN:HD22	2.16	0.57
1:C:207:PHE:CZ	1:C:391:ASP:HB2	2.40	0.57
1:E:385:ARG:HH11	1:E:385:ARG:HB3	1.69	0.57
1:A:79:ARG:HE	1:A:94:ASN:HD21	1.53	0.57
1:A:189:GLU:C	1:A:190:LEU:HD12	2.29	0.57
1:D:59:ASN:HD22	1:D:195:ILE:HD12	1.69	0.57
1:D:13:PHE:HB2	1:D:316:VAL:HB	1.86	0.57
1:E:218:ASN:ND2	1:E:220:ARG:HB2	2.19	0.57
1:F:214:THR:OG1	1:F:216:GLU:HG2	2.03	0.57
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.68	0.57
1:C:58:PRO:HD3	1:C:119:ASN:ND2	2.20	0.57
1:D:274:LEU:C	1:D:274:LEU:HD12	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:N	1:A:50:ARG:HH22	2.02	0.57
1:B:79:ARG:NH1	1:B:94:ASN:ND2	2.50	0.57
1:D:384:GLN:NE2	1:D:386:GLU:HB2	2.20	0.57
1:B:247:LEU:O	1:B:249:ILE:HG13	2.04	0.57
1:C:319:ILE:N	1:C:319:ILE:HD12	2.19	0.57
1:E:87:ASN:HD22	1:E:88:ASP:H	1.53	0.57
1:F:362:GLU:O	1:F:366:GLN:HG3	2.05	0.57
1:C:32:LEU:CD1	1:C:50:ARG:HH22	2.18	0.57
1:F:9:ASN:C	1:F:9:ASN:ND2	2.61	0.57
1:D:50:ARG:NH2	2:D:446:HOH:O	2.35	0.56
1:F:151:GLN:HG2	1:F:174:PHE:CZ	2.40	0.56
1:F:251:LEU:C	1:F:251:LEU:HD12	2.30	0.56
1:E:132:PRO:HA	2:E:442:HOH:O	2.06	0.56
1:E:206:SER:H	1:E:209:THR:HG22	1.70	0.56
1:F:32:LEU:HD22	1:F:50:ARG:NH2	2.20	0.56
1:F:306:ARG:HD3	1:F:308:ARG:NH1	2.19	0.56
1:E:207:ARG:NH2	1:E:222:ARG:HA	2.19	0.56
1:A:356:ASN:HD22	1:A:359:ARG:CD	2.19	0.56
1:E:375:GLN:O	1:E:379:ARG:HB2	2.05	0.56
1:F:254:ASN:HB3	1:F:334:ASN:O	2.06	0.56
1:F:262:LEU:HD21	1:F:323:TYR:HB3	1.88	0.56
1:F:380:LEU:C	1:F:382:LYS:H	2.14	0.56
1:B:9:ASN:C	1:B:9:ASN:HD22	2.12	0.56
1:A:67:ALA:C	1:A:69:ALA:H	2.14	0.56
1:C:146:GLN:NE2	1:C:146:GLN:C	2.63	0.56
1:E:219:LEU:HD23	1:E:219:LEU:H	1.69	0.56
1:B:364:GLN:H	1:B:364:GLN:CD	2.14	0.56
1:D:319:ILE:N	1:D:319:ILE:HD12	2.21	0.56
1:F:9:ASN:ND2	1:F:11:PHE:H	2.03	0.56
1:F:32:LEU:HD21	1:F:50:ARG:HD2	1.88	0.56
1:F:195:ASN:ND2	1:F:198:SER:N	2.54	0.56
1:B:190:LEU:HD23	1:C:368:LEU:HD21	1.88	0.56
1:B:331:SER:O	1:B:332:ASN:C	2.49	0.56
1:C:61:ILE:HG13	1:C:111:LEU:O	2.05	0.56
1:E:222:ARG:HH22	1:E:240:LYS:HG3	1.69	0.56
1:C:196:LEU:CD2	1:C:230:SER:HB2	2.35	0.56
1:D:38:LYS:HD3	1:D:38:LYS:C	2.30	0.56
1:B:4:ARG:HB2	1:B:306:ARG:O	2.06	0.55
1:C:39:ARG:HG2	1:C:39:ARG:NH1	2.21	0.55
1:E:173:LEU:O	1:F:371:PRO:HD2	2.06	0.55
1:E:250:PHE:C	1:E:250:PHE:CD2	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:SER:OG	1:C:337:ALA:HB3	2.06	0.55
1:C:302:LEU:HD12	1:C:302:LEU:H	1.72	0.55
1:D:9:ASN:ND2	1:D:11:PHE:H	2.04	0.55
1:F:207:PHE:CZ	1:F:391:ASP:HB2	2.42	0.55
1:C:50:ARG:HB3	1:C:50:ARG:NH2	2.14	0.55
1:C:189:GLU:CD	1:C:189:GLU:H	2.13	0.55
1:E:26:GLN:H	1:E:26:GLN:HE21	1.53	0.55
1:B:261:LEU:HD23	1:B:261:LEU:H	1.70	0.55
1:C:35:ARG:CZ	1:C:38:LYS:HG3	2.37	0.55
1:B:218:ASN:HD22	1:B:220:ARG:N	2.05	0.55
1:F:73:LEU:HG	1:F:124:TRP:NE1	2.21	0.55
1:A:313:GLU:O	1:A:314:ASP:HB2	2.06	0.55
1:C:112:VAL:HG12	1:C:113:ASN:N	2.21	0.55
1:B:265:HIS:HB2	1:B:348:ASN:O	2.07	0.55
1:A:285:LEU:HD22	1:A:286:VAL:N	2.22	0.55
1:A:285:LEU:HD21	1:A:323:TYR:HB3	1.87	0.55
1:B:280:ASP:HB2	1:B:330:THR:OG1	2.06	0.55
1:B:382:LYS:HE2	1:B:385:ARG:CZ	2.37	0.55
1:D:274:LEU:C	1:D:274:LEU:CD1	2.80	0.55
1:E:331:SER:O	1:E:332:ASN:C	2.50	0.55
1:B:26:GLN:NE2	1:B:26:GLN:N	2.44	0.55
1:B:102:ARG:H	1:B:243:GLN:NE2	2.05	0.55
1:C:207:PHE:HB3	1:C:237:ALA:CB	2.37	0.55
1:A:37:ASN:H	1:A:37:ASN:ND2	1.98	0.54
1:A:59:ASN:HA	1:A:195:ILE:CD1	2.36	0.54
1:B:218:ASN:HD22	1:B:220:ARG:H	1.53	0.54
1:C:102:ARG:CB	1:C:220:GLN:HE21	2.19	0.54
1:D:38:LYS:HD3	1:D:39:ARG:N	2.22	0.54
1:E:32:LEU:HD11	1:E:50:ARG:NH2	2.21	0.54
1:F:89:ASP:CG	1:F:90:ARG:N	2.65	0.54
1:D:221:SER:O	1:D:222:ARG:HG3	2.07	0.54
1:D:237:THR:OG1	1:D:240:LYS:HE2	2.07	0.54
1:A:356:ASN:HD22	1:A:359:ARG:CG	2.20	0.54
1:B:257:ASN:N	1:B:257:ASN:ND2	2.56	0.54
1:C:378:GLU:HG2	1:C:382:LYS:HG3	1.89	0.54
1:D:365:VAL:HG21	1:F:110:TYR:CE2	2.42	0.54
1:E:270:ALA:H	1:E:345:ASN:ND2	2.04	0.54
1:F:302:LEU:H	1:F:302:LEU:CD2	2.19	0.54
1:A:224:PRO:HG2	1:A:227:SER:HB2	1.90	0.54
1:C:56:SER:OG	1:C:120:LEU:HB3	2.07	0.54
1:F:170:ASN:ND2	1:F:175:GLY:H	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HD3	1:A:31:ARG:CG	2.34	0.54
1:E:85:VAL:HG23	1:F:360:GLN:HB3	1.88	0.54
1:E:219:LEU:HB2	1:E:236:ILE:HD11	1.89	0.54
1:F:102:ARG:H	1:F:220:GLN:NE2	2.06	0.54
1:F:382:LYS:NZ	1:F:385:ARG:HH21	2.05	0.54
1:D:67:ALA:C	1:D:69:ALA:H	2.16	0.54
1:D:130:ASN:C	1:E:45:ASN:HD22	2.15	0.54
1:E:385:ARG:NH1	1:E:385:ARG:HB3	2.22	0.54
1:C:166:PHE:CD2	1:C:169:ILE:HD11	2.43	0.54
1:E:241:ASN:OD1	1:E:243:GLN:HB2	2.07	0.54
1:B:31:ARG:HE	1:B:53:GLN:NE2	2.05	0.54
1:B:215:GLU:HB3	1:B:216:PRO:HD2	1.90	0.54
1:E:50:ARG:NH1	2:E:450:HOH:O	2.41	0.54
1:C:205:ASN:ND2	1:C:389:PHE:HB2	2.23	0.54
1:E:261:LEU:HD22	1:E:392:ALA:HB2	1.89	0.54
1:F:80:ALA:O	1:F:95:LEU:N	2.40	0.54
1:F:331:SER:O	1:F:332:ASN:C	2.50	0.54
1:A:9:ASN:C	1:A:9:ASN:HD22	2.15	0.53
1:B:313:GLU:O	1:B:314:ASP:HB2	2.08	0.53
1:C:216:GLU:CD	1:C:216:GLU:H	2.15	0.53
1:C:364:GLN:CD	1:C:364:GLN:H	2.17	0.53
1:F:14:ARG:C	1:F:16:SER:H	2.16	0.53
1:B:219:LEU:HD23	1:B:253:SER:HB2	1.91	0.53
1:D:55:GLN:HA	1:D:120:LEU:O	2.08	0.53
1:E:102:ARG:CB	1:E:243:GLN:HE21	2.18	0.53
1:F:260:ILE:CD1	1:F:311:LEU:HD11	2.38	0.53
1:B:110:TYR:CE2	1:C:365:VAL:HG21	2.43	0.53
1:C:246:LYS:H	1:C:345:ASN:HD22	1.57	0.53
1:B:219:LEU:HD21	1:B:253:SER:N	2.23	0.53
1:F:189:GLU:O	1:F:190:LEU:C	2.52	0.53
1:A:224:PRO:HD3	1:A:234:PHE:CE2	2.44	0.53
1:B:159:GLU:OE2	1:B:166:PHE:HB2	2.09	0.53
1:C:33:LEU:O	1:C:50:ARG:NH2	2.42	0.53
1:E:218:ASN:HD22	1:E:220:ARG:N	2.00	0.53
1:F:246:LYS:H	1:F:345:ASN:HD22	1.57	0.53
1:B:102:ARG:H	1:B:243:GLN:HE22	1.57	0.53
1:D:73:LEU:HD22	1:D:124:TRP:CG	2.43	0.53
1:C:202:ILE:HG12	1:C:210:PHE:O	2.09	0.53
1:C:54:PHE:HE2	1:C:120:LEU:HD23	1.74	0.53
1:D:222:ARG:HG3	1:D:222:ARG:NH2	2.23	0.53
1:F:143:THR:HG21	1:F:185:GLY:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:GLN:HG2	1:F:174:PHE:CE1	2.43	0.53
1:F:218:ASN:HB3	1:F:221:LEU:HB2	1.91	0.53
1:B:250:PHE:C	1:B:250:PHE:CD2	2.86	0.52
1:D:237:THR:H	1:D:240:LYS:CE	2.21	0.52
1:C:59:ASN:HD21	1:C:116:ASP:CG	2.17	0.52
1:F:25:ASN:OD1	1:F:27:ASN:N	2.42	0.52
1:F:386:GLU:HB3	1:F:390:VAL:HG12	1.91	0.52
1:B:274:LEU:HD22	1:B:335:PHE:CD2	2.44	0.52
1:C:240:LEU:HD12	1:C:388:TYR:N	2.23	0.52
1:D:110:TYR:CE2	1:E:365:VAL:HG21	2.43	0.52
1:B:283:ILE:CD1	1:B:311:LEU:HD11	2.39	0.52
1:C:15:SER:HB2	1:C:31:ARG:HH12	1.75	0.52
1:C:39:ARG:HD2	1:C:40:SER:OG	2.10	0.52
1:C:258:ALA:HB2	1:C:333:LEU:HD22	1.90	0.52
1:D:40:SER:C	1:D:42:GLN:H	2.15	0.52
1:E:269:LYS:H	1:E:345:ASN:ND2	2.07	0.52
1:A:277:ASN:O	1:A:277:ASN:ND2	2.43	0.52
1:C:62:LEU:HD23	1:C:186:VAL:O	2.09	0.52
1:D:140:LEU:HD11	1:E:358:VAL:HG22	1.91	0.52
1:E:110:TYR:CE2	1:F:365:VAL:HG21	2.44	0.52
1:F:115:HIS:CE1	1:F:118:GLN:H	2.27	0.52
1:A:285:LEU:HD22	1:A:286:VAL:H	1.73	0.52
1:B:208:LYS:HG3	1:B:208:LYS:O	2.10	0.52
1:E:189:GLU:C	1:E:190:LEU:HG	2.35	0.52
1:A:218:ASN:HD22	1:A:220:ARG:N	2.02	0.52
1:B:222:ARG:HH22	1:B:240:LYS:HG3	1.74	0.52
1:B:258:GLU:H	1:B:332:ASN:ND2	2.08	0.52
1:C:247:ALA:H	1:C:345:ASN:ND2	2.08	0.52
1:F:189:GLU:O	1:F:190:LEU:HD23	2.10	0.52
1:E:6:ASP:O	1:E:7:GLU:HB2	2.09	0.52
1:C:147:GLN:HB3	1:C:151:GLN:OE1	2.10	0.52
1:D:10:PRO:HB2	1:D:40:SER:HB2	1.92	0.52
1:D:223:ASN:N	1:D:223:ASN:HD22	2.08	0.52
1:D:261:LEU:HD22	1:D:392:ALA:HB2	1.92	0.52
1:A:58:PRO:HD3	1:A:119:ASN:ND2	2.24	0.51
1:A:250:PHE:C	1:A:250:PHE:CD2	2.87	0.51
1:B:6:ASP:O	1:B:7:GLU:CB	2.58	0.51
1:D:34:GLN:HE22	1:D:38:LYS:HE2	1.75	0.51
1:A:69:ALA:CB	1:A:128:PRO:HA	2.40	0.51
1:A:373:SER:H	1:A:376:ASP:HB2	1.75	0.51
1:B:68:ASP:OD2	1:B:135:TYR:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ARG:HG3	1:D:207:ARG:NH1	2.25	0.51
1:D:356:ASN:C	1:D:356:ASN:HD22	2.18	0.51
1:B:170:ASN:O	1:B:175:GLY:N	2.42	0.51
1:F:240:LEU:HD13	1:F:351:ALA:O	2.10	0.51
1:A:170:ASN:ND2	1:A:174:PHE:HB2	2.26	0.51
1:C:385:ARG:HG2	1:C:385:ARG:HH11	1.75	0.51
1:C:320:PRO:HB2	1:C:323:TYR:CD1	2.45	0.51
1:E:377:VAL:O	1:E:381:LEU:HG	2.10	0.51
1:E:193:GLU:OE2	1:E:196:ARG:NH1	2.43	0.51
1:F:30:ILE:HG12	1:F:54:PHE:CD1	2.45	0.51
1:E:277:ASN:HB3	1:E:334:ASN:ND2	2.22	0.51
1:E:387:SER:O	1:E:389:PHE:N	2.40	0.51
1:B:59:ASN:HA	1:B:195:ILE:HD11	1.92	0.51
1:E:259:GLY:O	1:E:392:ALA:HB3	2.10	0.51
1:D:17:ASN:HD22	1:D:18:SER:N	2.08	0.51
1:B:30:ILE:HG12	1:B:54:PHE:HD1	1.77	0.51
1:B:382:LYS:NZ	1:B:385:ARG:HH12	2.06	0.51
1:F:48:ASP:OD1	1:F:132:PRO:HB3	2.11	0.51
1:A:35:ARG:HG3	1:A:50:ARG:HH22	1.74	0.50
1:E:219:LEU:HB3	1:E:236:ILE:HG12	1.93	0.50
1:E:235:GLU:C	1:E:236:ILE:HD13	2.37	0.50
1:F:49:TYR:O	1:F:50:ARG:HG2	2.11	0.50
1:D:17:ASN:C	1:D:17:ASN:ND2	2.64	0.50
1:D:206:SER:O	1:D:207:ARG:C	2.54	0.50
1:F:169:ILE:HG13	1:F:170:ASN:N	2.26	0.50
1:E:196:ARG:C	1:E:198:LEU:H	2.19	0.50
1:F:31:ARG:HH21	1:F:53:GLN:CD	2.20	0.50
1:F:119:ASN:N	1:F:119:ASN:HD22	2.09	0.50
1:C:102:ARG:H	1:C:220:GLN:HE22	1.59	0.50
1:C:122:MET:HE3	1:C:124:TRP:NE1	2.26	0.50
1:F:87:ASN:C	1:F:87:ASN:HD22	2.20	0.50
1:F:170:ASN:HD22	1:F:170:ASN:C	2.19	0.50
1:F:189:GLU:O	1:F:190:LEU:O	2.30	0.50
1:F:242:HIS:HB3	1:F:349:PHE:CD1	2.47	0.50
1:C:99:ASP:HA	1:C:195:ASN:HA	1.94	0.50
1:E:6:ASP:C	1:E:8:ASN:H	2.19	0.50
1:E:258:GLU:H	1:E:332:ASN:ND2	2.10	0.50
1:F:14:ARG:CG	1:F:16:SER:HB3	2.38	0.50
1:A:363:ARG:HG2	1:A:378:GLU:OE1	2.11	0.50
1:C:80:ALA:HB2	1:C:120:LEU:CD1	2.41	0.50
1:C:215:PRO:HD2	1:C:216:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LYS:HB3	1:C:303:GLU:HB2	1.93	0.50
1:E:57:LYS:HB3	1:E:58:PRO:HD2	1.93	0.50
1:B:168:GLU:O	1:B:172:VAL:HG23	2.12	0.50
1:C:261:GLU:CD	1:C:308:ARG:HH21	2.20	0.50
1:A:176:GLU:HB2	2:A:444:HOH:O	2.12	0.49
1:C:61:ILE:HG13	1:C:112:VAL:HG22	1.93	0.49
1:D:9:ASN:HD22	1:D:11:PHE:H	1.60	0.49
1:F:261:GLU:HB2	1:F:326:VAL:HG12	1.94	0.49
1:A:222:ARG:NH2	1:A:222:ARG:HG3	2.27	0.49
1:A:267:ASN:HB3	1:A:345:ASN:HD21	1.77	0.49
1:B:312:SER:O	1:B:315:ASP:HB2	2.12	0.49
1:B:379:ARG:HG3	1:B:379:ARG:HH11	1.77	0.49
1:C:34:GLN:OE1	1:C:39:ARG:HG2	2.12	0.49
1:D:34:GLN:NE2	1:D:38:LYS:HE2	2.27	0.49
1:D:122:MET:HE3	1:D:124:TRP:NE1	2.18	0.49
1:E:230:PHE:CZ	1:E:391:ASP:HB2	2.47	0.49
1:F:196:LEU:HD21	1:F:230:SER:N	2.27	0.49
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.76	0.49
1:D:244:LEU:HG	1:D:249:ILE:O	2.12	0.49
1:C:79:ARG:HD2	1:C:94:ASN:ND2	2.24	0.49
1:E:102:ARG:H	1:E:243:GLN:HE22	1.61	0.49
1:F:205:ASN:ND2	1:F:389:PHE:HB2	2.27	0.49
1:F:32:LEU:HD22	1:F:50:ARG:HH21	1.78	0.49
1:F:101:GLN:HG2	1:F:102:ARG:N	2.27	0.49
1:A:380:LEU:HD12	1:C:172:VAL:HB	1.94	0.49
1:D:224:PRO:HG2	1:D:227:SER:HB2	1.93	0.49
1:E:222:ARG:NH1	1:E:236:ILE:HD12	2.27	0.49
1:E:269:LYS:H	1:E:345:ASN:HD22	1.60	0.49
1:F:347:ARG:NH1	2:F:417:HOH:O	2.41	0.49
1:A:53:GLN:HE22	1:A:314:ASP:HB3	1.77	0.49
1:B:238:PRO:HB3	1:B:245:ARG:HA	1.93	0.49
1:B:87:ASN:HD22	1:B:88:ASP:H	1.59	0.49
1:E:247:LEU:O	1:E:249:ILE:HG13	2.13	0.49
1:F:89:ASP:OD1	1:F:90:ARG:N	2.45	0.49
1:A:147:GLN:OE1	1:B:304:VAL:HG22	2.13	0.49
1:D:184:GLU:HG3	2:D:450:HOH:O	2.11	0.49
1:E:219:LEU:HA	1:E:236:ILE:HD11	1.94	0.49
1:E:284:GLU:HB2	1:E:326:VAL:CG1	2.43	0.49
1:A:59:ASN:ND2	1:A:195:ILE:HD12	2.27	0.48
1:B:277:ASN:CB	1:B:334:ASN:HD22	2.26	0.48
1:C:386:GLU:CB	1:C:390:VAL:HG12	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASN:HD22	1:A:87:ASN:C	2.18	0.48
1:A:131:LYS:HG3	1:A:134:ARG:HB2	1.94	0.48
1:C:205:ASN:HD21	1:C:389:PHE:HB2	1.78	0.48
1:D:54:PHE:CD2	1:D:122:MET:HE2	2.48	0.48
1:E:9:ASN:ND2	1:E:11:PHE:H	2.12	0.48
1:A:55:GLN:HA	1:A:120:LEU:O	2.13	0.48
1:C:61:ILE:CG1	1:C:112:VAL:HG22	2.43	0.48
1:C:238:LEU:HD21	1:C:390:VAL:HG22	1.96	0.48
1:F:60:THR:O	1:F:112:VAL:HG13	2.13	0.48
1:F:261:GLU:HB2	1:F:326:VAL:CG1	2.43	0.48
1:A:270:ALA:H	1:A:345:ASN:ND2	2.09	0.48
1:F:125:LEU:HD22	1:F:338:PHE:CD2	2.49	0.48
1:A:206:SER:O	1:A:207:ARG:C	2.57	0.48
1:D:192:LYS:O	1:D:196:ARG:HB2	2.13	0.48
1:D:322:ALA:HB3	1:F:68:ASP:HB3	1.94	0.48
1:C:190:LEU:O	1:C:190:LEU:HD23	2.14	0.48
1:D:250:PHE:C	1:D:250:PHE:CD2	2.92	0.48
1:F:215:PRO:O	1:F:222:ARG:HB2	2.13	0.48
1:B:363:ARG:NH1	1:B:378:GLU:OE2	2.47	0.48
1:E:101:GLN:NE2	1:E:216:PRO:HD3	2.29	0.48
1:F:225:ASP:OD2	1:F:343:GLU:HB2	2.13	0.48
1:A:120:LEU:CD2	1:A:122:MET:HE2	2.36	0.48
1:C:72:LEU:HB3	1:C:125:LEU:HB3	1.95	0.48
1:E:160:THR:HG21	1:F:392:ALA:HA	1.96	0.48
1:F:80:ALA:HB2	1:F:120:LEU:CD1	2.44	0.48
1:F:254:ASN:O	1:F:313:GLU:HG3	2.14	0.48
1:A:223:ASN:N	1:A:223:ASN:HD22	2.11	0.47
1:D:10:PRO:HB2	1:D:40:SER:CB	2.44	0.47
1:D:40:SER:C	1:D:42:GLN:N	2.70	0.47
1:F:189:GLU:C	1:F:190:LEU:HD23	2.39	0.47
1:A:288:ILE:HG21	1:A:302:LEU:HD13	1.95	0.47
1:A:359:ARG:HB2	1:A:359:ARG:HH11	1.79	0.47
1:B:49:TYR:O	1:B:50:ARG:HG2	2.14	0.47
1:B:81:ILE:HD11	1:B:199:SER:HB3	1.94	0.47
1:C:100:ALA:HB3	1:C:194:PHE:CE2	2.49	0.47
1:C:189:GLU:O	1:C:190:LEU:C	2.57	0.47
1:F:13:PHE:CZ	1:F:39:ARG:HG3	2.49	0.47
1:F:15:SER:CB	1:F:314:ASP:HB3	2.44	0.47
1:F:25:ASN:OD1	1:F:25:ASN:C	2.58	0.47
1:F:191:ASP:OD2	1:F:192:GLU:N	2.46	0.47
1:F:253:ILE:HD11	1:F:311:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:CE2	1:A:186:VAL:HB	2.49	0.47
1:E:261:LEU:N	1:E:261:LEU:HD23	2.29	0.47
1:B:23:PHE:CD1	1:B:23:PHE:C	2.92	0.47
1:B:319:ILE:HD12	1:B:319:ILE:N	2.29	0.47
1:C:76:LEU:HD11	1:C:123:ILE:HG12	1.95	0.47
1:C:85:VAL:HG13	1:C:108:THR:HB	1.96	0.47
1:C:306:ARG:HB3	1:C:308:ARG:HH11	1.79	0.47
1:D:57:LYS:HB3	1:D:58:PRO:HD2	1.97	0.47
1:D:131:LYS:HG3	1:D:134:ARG:HB2	1.96	0.47
1:D:378:GLU:O	1:D:382:LYS:HB2	2.14	0.47
1:E:321:ALA:O	1:E:322:ALA:HB3	2.13	0.47
1:F:380:LEU:C	1:F:380:LEU:HD23	2.39	0.47
1:B:214:ASP:OD1	1:B:215:GLU:HG3	2.14	0.47
1:F:6:ASP:C	1:F:8:ASN:N	2.73	0.47
1:C:259:ASN:ND2	1:C:330:THR:CG2	2.78	0.47
1:D:359:ARG:HH11	1:D:382:LYS:HD2	1.80	0.47
1:E:32:LEU:HD23	1:E:52:VAL:HG22	1.96	0.47
1:E:80:ALA:HB2	1:E:120:LEU:HD22	1.97	0.47
1:E:146:GLN:NE2	1:E:146:GLN:C	2.73	0.47
1:F:71:PHE:HE2	1:F:126:ALA:HB2	1.80	0.47
1:F:73:LEU:HG	1:F:124:TRP:CD1	2.50	0.47
1:F:85:VAL:CG1	1:F:108:THR:HG22	2.44	0.47
1:A:59:ASN:CA	1:A:195:ILE:HD11	2.42	0.47
1:A:73:LEU:HD22	1:A:124:TRP:CG	2.49	0.47
1:A:210:ILE:HD11	1:A:236:ILE:CG2	2.45	0.47
1:A:217:PHE:N	1:A:217:PHE:CD1	2.82	0.47
1:A:249:ILE:HA	1:A:339:GLY:O	2.14	0.47
1:B:23:PHE:CD2	1:B:186:VAL:HG22	2.50	0.47
1:B:382:LYS:HG3	1:B:385:ARG:NH1	2.29	0.47
1:C:6:ASP:C	1:C:8:ASN:H	2.23	0.47
1:C:146:GLN:C	1:C:146:GLN:HE21	2.21	0.47
1:D:306:ARG:NH2	2:D:480:HOH:O	2.48	0.47
1:E:306:ARG:HD3	2:E:451:HOH:O	2.14	0.47
1:F:184:GLU:HG2	1:F:188:VAL:HG12	1.96	0.47
1:F:257:ASP:O	1:F:258:ALA:HB2	2.14	0.47
1:F:357:VAL:O	1:F:360:GLN:HB2	2.15	0.47
1:F:384:GLN:NE2	1:F:386:GLU:HB2	2.29	0.47
1:A:356:ASN:HD22	1:A:359:ARG:HD3	1.78	0.47
1:B:267:ASN:HB3	1:B:345:ASN:HD21	1.79	0.47
1:F:247:ALA:H	1:F:345:ASN:ND2	2.12	0.47
1:F:256:GLY:HA3	1:F:332:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD21	1:A:122:MET:CE	2.37	0.47
1:B:83:THR:HG21	1:B:110:TYR:CE2	2.50	0.47
1:B:154:SER:OG	1:B:157:ILE:HD13	2.14	0.47
1:C:258:ALA:CB	1:C:333:LEU:HD22	2.45	0.47
1:C:320:PRO:HB2	1:C:323:TYR:CG	2.50	0.47
1:D:69:ALA:O	1:D:105:ALA:HA	2.15	0.47
1:D:87:ASN:HD22	1:D:87:ASN:C	2.20	0.47
1:D:228:ASN:C	1:D:228:ASN:OD1	2.57	0.47
1:E:219:LEU:CB	1:E:236:ILE:HD11	2.45	0.47
1:E:319:ILE:HG21	1:E:325:PHE:CD1	2.50	0.47
1:F:266:LYS:HB3	1:F:303:GLU:HB2	1.97	0.47
1:B:165:GLU:HG3	1:B:167:GLU:HG3	1.96	0.47
1:B:281:ALA:HB2	1:B:333:LEU:HD22	1.97	0.47
1:C:227:PHE:C	1:C:227:PHE:HD2	2.21	0.47
1:C:266:LYS:HE3	1:C:305:GLN:OE1	2.14	0.47
1:D:285:LEU:HD22	1:D:286:VAL:N	2.30	0.47
1:F:61:ILE:HB	1:F:112:VAL:HG22	1.97	0.47
1:C:64:PRO:HG3	1:C:110:TYR:CD1	2.50	0.46
1:C:73:LEU:HG	1:C:124:TRP:NE1	2.29	0.46
1:F:55:GLN:HA	1:F:120:LEU:O	2.14	0.46
1:F:254:ASN:C	1:F:254:ASN:HD22	2.23	0.46
1:F:321:ALA:O	1:F:322:ALA:HB3	2.14	0.46
1:A:356:ASN:HD22	1:A:359:ARG:HG2	1.79	0.46
1:A:371:PRO:O	1:A:372:GLY:O	2.33	0.46
1:B:34:GLN:HE21	1:B:39:ARG:HB2	1.80	0.46
1:B:37:ASN:N	1:B:37:ASN:ND2	2.61	0.46
1:C:385:ARG:HG2	1:C:385:ARG:NH1	2.28	0.46
1:D:59:ASN:HA	1:D:195:ILE:CD1	2.45	0.46
1:D:380:LEU:HD11	1:F:169:ILE:HA	1.96	0.46
1:E:260:ALA:HA	1:E:392:ALA:H	1.80	0.46
1:F:32:LEU:CD2	1:F:50:ARG:HD2	2.45	0.46
1:F:353:GLU:OE2	1:F:385:ARG:HA	2.15	0.46
1:A:79:ARG:HB2	1:A:115:HIS:CE1	2.51	0.46
1:A:110:TYR:CE2	1:B:365:VAL:HG21	2.50	0.46
1:C:111:LEU:HD21	1:C:120:LEU:HD21	1.97	0.46
1:E:154:SER:HB3	1:F:308:ARG:NH2	2.31	0.46
2:A:430:HOH:O	1:B:45:ASN:HB2	2.14	0.46
1:C:15:SER:HB3	1:C:314:ASP:O	2.15	0.46
1:C:33:LEU:HD12	1:C:34:GLN:H	1.81	0.46
1:C:260:ILE:O	1:C:308:ARG:HA	2.15	0.46
1:D:13:PHE:HB2	1:D:316:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:ASN:HB3	1:D:359:ARG:HG2	1.96	0.46
1:F:33:LEU:O	1:F:50:ARG:NH2	2.39	0.46
1:A:47:ARG:HH12	1:A:132:PRO:CB	2.28	0.46
1:C:58:PRO:HB3	1:C:116:ASP:HA	1.97	0.46
1:C:89:ASP:CG	1:C:90:ARG:N	2.73	0.46
1:A:222:ARG:HG3	1:A:222:ARG:HH21	1.80	0.46
1:B:79:ARG:HB2	1:B:115:HIS:NE2	2.31	0.46
1:C:215:PRO:HB3	1:C:222:ARG:HA	1.97	0.46
1:C:362:GLU:O	1:C:366:GLN:HG3	2.16	0.46
1:F:170:ASN:HD22	1:F:175:GLY:H	1.62	0.46
1:C:257:ASP:O	1:C:333:LEU:HD13	2.16	0.46
1:D:9:ASN:C	1:D:9:ASN:ND2	2.68	0.46
1:E:19:PHE:CZ	1:E:33:LEU:HD13	2.51	0.46
1:E:33:LEU:O	1:E:50:ARG:NH2	2.48	0.46
1:F:82:LEU:HD13	1:F:111:LEU:HD13	1.97	0.46
1:F:147:GLN:HG2	1:F:151:GLN:OE1	2.16	0.46
1:F:227:PHE:C	1:F:227:PHE:HD2	2.23	0.46
1:D:80:ALA:HB2	1:D:120:LEU:CD1	2.46	0.46
1:D:392:ALA:HA	1:F:160:THR:HG21	1.98	0.46
1:E:129:VAL:O	1:F:45:ASN:ND2	2.48	0.46
1:A:7:GLU:OE2	1:A:14:ARG:NH1	2.49	0.46
1:A:200:ARG:O	1:A:201:ARG:HB3	2.14	0.46
1:B:103:ILE:O	1:B:104:PRO:C	2.57	0.46
1:B:304:VAL:HG23	1:B:304:VAL:O	2.16	0.46
1:C:235:GLU:HG2	1:C:236:GLY:N	2.31	0.46
1:F:226:ILE:HA	1:F:339:GLY:O	2.16	0.46
1:A:319:ILE:HD13	1:A:325:PHE:CZ	2.52	0.46
1:B:206:SER:O	1:B:209:THR:HG22	2.16	0.46
1:C:82:LEU:HD13	1:C:111:LEU:HD13	1.98	0.46
1:D:274:LEU:HD22	1:D:335:PHE:CE2	2.51	0.46
1:E:166:PHE:HZ	1:E:170:ASN:HD22	1.61	0.46
1:F:14:ARG:HA	1:F:315:ASP:OD2	2.15	0.46
1:C:377:VAL:O	1:C:381:LEU:HG	2.17	0.45
1:D:267:ASN:HB3	1:D:345:ASN:HD21	1.81	0.45
1:D:23:PHE:HZ	1:D:185:GLY:HA3	1.81	0.45
1:A:210:ILE:HD11	1:A:236:ILE:HG23	1.99	0.45
1:B:30:ILE:HG12	1:B:54:PHE:CD1	2.52	0.45
1:D:226:TYR:HB3	1:D:388:TYR:CD1	2.51	0.45
1:D:320:PRO:HB2	1:D:323:TYR:CD1	2.51	0.45
1:E:68:ASP:OD2	1:E:135:TYR:HB2	2.16	0.45
1:F:166:PHE:CD2	1:F:169:ILE:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LEU:C	1:C:380:LEU:HD23	2.40	0.45
1:E:277:ASN:ND2	2:E:460:HOH:O	2.50	0.45
1:A:384:GLN:NE2	1:A:386:GLU:HB2	2.32	0.45
1:D:274:LEU:HD22	1:D:335:PHE:CD2	2.52	0.45
1:E:167:GLU:HG3	1:E:168:GLU:N	2.31	0.45
1:A:183:GLN:CG	1:A:188:VAL:CG1	2.91	0.45
1:E:220:ARG:C	1:E:222:ARG:N	2.74	0.45
1:E:222:ARG:CZ	1:E:236:ILE:HD12	2.47	0.45
1:E:319:ILE:HD12	1:E:319:ILE:N	2.30	0.45
1:F:215:PRO:HB3	1:F:222:ARG:HA	1.99	0.45
1:A:150:LEU:HD21	1:B:350:LEU:HD13	1.99	0.45
1:C:25:ASN:OD1	1:C:25:ASN:C	2.59	0.45
1:E:6:ASP:HB2	1:E:7:GLU:OE1	2.17	0.45
1:E:49:TYR:CZ	1:E:340:ILE:HD12	2.52	0.45
1:A:40:SER:C	1:A:42:GLN:H	2.25	0.45
1:A:74:PHE:HE2	1:A:219:LEU:HD13	1.81	0.45
1:B:6:ASP:O	1:B:6:ASP:OD1	2.35	0.45
1:B:23:PHE:CD1	1:B:24:GLU:N	2.85	0.45
1:C:65:HIS:HB2	1:C:138:PHE:O	2.17	0.45
1:C:81:ILE:HG13	1:C:114:PRO:HG3	1.98	0.45
1:E:30:ILE:HG12	1:E:54:PHE:HD1	1.81	0.45
1:E:226:TYR:HB2	1:E:233:PHE:HB3	1.99	0.45
1:F:229:SER:OG	1:F:337:ALA:HB3	2.17	0.45
1:B:85:VAL:HG13	1:B:108:THR:HB	1.98	0.45
1:C:119:ASN:N	1:C:119:ASN:ND2	2.65	0.45
1:E:9:ASN:C	1:E:9:ASN:ND2	2.73	0.45
1:B:32:LEU:CD1	1:B:50:ARG:CZ	2.92	0.45
1:C:76:LEU:HB2	1:C:121:LYS:O	2.17	0.45
1:D:217:PHE:CD1	1:D:217:PHE:N	2.85	0.45
1:E:73:LEU:HG	1:E:124:TRP:CD1	2.52	0.45
1:E:265:HIS:HB2	1:E:348:ASN:O	2.16	0.45
1:F:214:THR:H	1:F:217:LYS:HE3	1.81	0.45
1:A:217:PHE:CZ	1:A:244:LEU:HD13	2.52	0.44
1:C:387:SER:O	1:C:389:PHE:N	2.44	0.44
1:D:37:ASN:HD22	1:D:37:ASN:N	2.12	0.44
1:D:114:PRO:HA	1:D:195:ILE:HD13	1.98	0.44
1:F:37:ASN:H	1:F:37:ASN:ND2	2.12	0.44
1:B:148:SER:OG	1:B:150:LEU:HB2	2.18	0.44
1:B:169:ILE:HA	1:C:380:LEU:HD11	2.00	0.44
1:B:184:GLU:O	1:B:185:GLY:O	2.36	0.44
1:B:387:SER:O	1:B:389:PHE:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:HD21	1:C:390:VAL:CG2	2.48	0.44
1:D:261:LEU:HD23	1:D:261:LEU:N	2.31	0.44
1:E:162:PHE:HB2	1:E:169:ILE:CD1	2.47	0.44
1:E:258:GLU:H	1:E:332:ASN:HD22	1.63	0.44
1:F:141:SER:O	1:F:148:SER:HB2	2.18	0.44
1:A:22:LEU:HD21	1:A:32:LEU:HD12	1.99	0.44
1:A:224:PRO:CG	1:A:227:SER:HB2	2.46	0.44
1:A:364:GLN:H	1:A:364:GLN:CD	2.23	0.44
1:B:32:LEU:HD23	1:B:52:VAL:HG22	1.99	0.44
1:C:6:ASP:C	1:C:8:ASN:N	2.73	0.44
1:D:8:ASN:O	1:D:8:ASN:ND2	2.50	0.44
1:D:79:ARG:HB2	1:D:115:HIS:CE1	2.53	0.44
1:F:58:PRO:HD3	1:F:119:ASN:ND2	2.31	0.44
1:F:96:HIS:O	1:F:99:ASP:HB2	2.17	0.44
1:A:357:VAL:O	1:A:360:GLN:HB2	2.17	0.44
1:C:111:LEU:CD2	1:C:122:MET:HE1	2.48	0.44
1:E:364:GLN:O	1:E:367:GLU:HB3	2.18	0.44
1:B:206:SER:O	1:B:208:LYS:N	2.51	0.44
1:D:263:LEU:HD13	1:D:351:ALA:O	2.17	0.44
1:D:306:ARG:HH21	1:D:306:ARG:HG3	1.82	0.44
1:F:37:ASN:N	1:F:37:ASN:ND2	2.65	0.44
1:A:281:ALA:HB2	1:A:333:LEU:HD22	2.00	0.44
1:B:59:ASN:HA	1:B:195:ILE:CD1	2.47	0.44
1:D:85:VAL:CG2	1:E:360:GLN:HB2	2.45	0.44
1:D:220:ARG:C	1:D:222:ARG:H	2.25	0.44
1:D:261:LEU:HD21	1:D:390:VAL:HG23	1.95	0.44
1:E:219:LEU:HB3	1:E:236:ILE:CG1	2.47	0.44
1:F:87:ASN:HD22	1:F:88:ASP:N	2.16	0.44
1:B:274:LEU:HD22	1:B:335:PHE:CE2	2.53	0.44
1:D:69:ALA:HB2	1:D:128:PRO:HA	2.00	0.44
1:E:13:PHE:HB2	1:E:316:VAL:HB	2.00	0.44
1:E:80:ALA:HB2	1:E:120:LEU:CD2	2.48	0.44
1:E:88:ASP:O	1:E:89:ASP:HB3	2.17	0.44
1:E:166:PHE:CZ	1:E:170:ASN:ND2	2.85	0.44
1:B:220:ARG:NH2	1:B:255:ASP:OD2	2.51	0.44
1:C:58:PRO:HB3	1:C:115:HIS:O	2.18	0.44
1:C:190:LEU:HD23	1:C:190:LEU:C	2.43	0.44
1:D:172:VAL:HG22	1:E:376:ASP:HB3	2.00	0.44
1:A:350:LEU:C	1:A:356:ASN:OD1	2.61	0.44
1:C:22:LEU:HB2	1:C:30:ILE:O	2.18	0.44
1:E:47:ARG:HH22	1:E:132:PRO:CB	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:GLN:HA	1:F:360:GLN:NE2	2.32	0.44
1:B:25:ASN:OD1	1:B:27:ASN:N	2.46	0.43
1:C:79:ARG:HG2	1:C:80:ALA:N	2.33	0.43
1:E:254:VAL:HG13	1:E:335:PHE:CE2	2.53	0.43
1:F:12:TYR:O	1:F:39:ARG:NH2	2.50	0.43
1:A:9:ASN:C	1:A:9:ASN:ND2	2.77	0.43
1:A:171:ARG:HD2	1:A:181:ARG:NH2	2.33	0.43
1:A:191:SER:O	1:A:192:LYS:C	2.58	0.43
1:A:361:ILE:CG2	1:A:365:VAL:HB	2.49	0.43
1:C:259:ASN:ND2	1:C:330:THR:HG21	2.33	0.43
1:D:304:VAL:O	1:D:304:VAL:HG23	2.17	0.43
1:F:79:ARG:HG2	1:F:80:ALA:N	2.33	0.43
1:A:387:SER:O	1:A:389:PHE:N	2.43	0.43
1:B:206:SER:H	1:B:209:THR:CG2	2.31	0.43
1:C:102:ARG:HB3	1:C:220:GLN:NE2	2.33	0.43
1:D:116:ASP:CG	1:D:192:LYS:HE2	2.43	0.43
1:D:285:LEU:CD2	1:D:323:TYR:HB3	2.45	0.43
1:E:206:SER:O	1:E:209:THR:HG22	2.17	0.43
1:E:219:LEU:CA	1:E:236:ILE:HD11	2.48	0.43
1:F:202:ILE:HG12	1:F:210:PHE:O	2.17	0.43
1:C:8:ASN:HD22	1:C:8:ASN:HA	1.52	0.43
1:D:75:VAL:HG21	1:D:95:LEU:HB3	2.00	0.43
1:B:274:LEU:HB3	1:B:317:PHE:O	2.19	0.43
1:C:379:ARG:HG3	1:C:379:ARG:NH1	2.31	0.43
1:D:210:ILE:HG23	1:D:211:SER:N	2.32	0.43
1:D:363:ARG:HG2	1:D:374:ALA:CB	2.46	0.43
1:E:159:GLU:OE2	1:E:166:PHE:HB2	2.18	0.43
1:B:219:LEU:HD11	1:B:235:GLU:HA	2.00	0.43
1:B:333:LEU:HG	1:B:334:ASN:N	2.33	0.43
1:C:170:ASN:ND2	1:C:170:ASN:O	2.51	0.43
1:C:196:LEU:HD13	1:C:213:ILE:HG12	2.00	0.43
1:E:116:ASP:OD2	1:E:192:LYS:HE3	2.19	0.43
1:F:9:ASN:HD21	1:F:11:PHE:HD2	1.65	0.43
1:B:203:LYS:HD3	1:B:215:GLU:OE2	2.18	0.43
1:D:170:ASN:HD22	1:D:174:PHE:HB2	1.84	0.43
1:F:254:ASN:C	1:F:254:ASN:ND2	2.77	0.43
1:B:353:GLU:HG3	1:B:385:ARG:O	2.19	0.43
1:E:222:ARG:NH1	1:E:236:ILE:CD1	2.82	0.43
1:F:8:ASN:HD22	1:F:8:ASN:HA	1.59	0.43
1:F:310:GLU:OE2	1:F:310:GLU:N	2.51	0.43
1:A:32:LEU:HD13	1:A:50:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ASP:HA	1:E:360:GLN:NE2	2.34	0.43
1:D:321:ALA:O	1:D:322:ALA:HB3	2.18	0.43
1:E:59:ASN:CA	1:E:195:ILE:HD11	2.43	0.43
1:E:277:ASN:CB	1:E:334:ASN:ND2	2.81	0.43
1:F:301:PRO:O	1:F:302:LEU:C	2.61	0.43
1:F:353:GLU:OE1	1:F:382:LYS:HE3	2.18	0.43
1:A:9:ASN:ND2	1:A:11:PHE:H	2.17	0.43
1:A:35:ARG:HG2	1:A:50:ARG:NH2	2.32	0.43
1:A:284:GLU:HG2	1:A:308:ARG:HG2	2.01	0.43
1:B:32:LEU:CD2	1:B:52:VAL:HG22	2.48	0.43
1:B:249:ILE:CG2	1:B:250:PHE:N	2.82	0.43
1:C:89:ASP:O	1:C:90:ARG:HB2	2.18	0.43
1:C:242:HIS:HB3	1:C:349:PHE:CD1	2.54	0.43
1:E:85:VAL:HG13	1:E:108:THR:HB	2.01	0.43
1:E:364:GLN:O	1:E:368:LEU:HD22	2.19	0.43
1:F:31:ARG:NE	1:F:53:GLN:NE2	2.66	0.43
1:F:112:VAL:HG12	1:F:113:ASN:N	2.33	0.43
1:B:11:PHE:CD1	1:B:43:LEU:HD21	2.54	0.42
1:B:11:PHE:CE1	1:B:43:LEU:HD21	2.52	0.42
1:C:252:VAL:HG21	1:C:336:LEU:HD23	2.01	0.42
1:A:368:LEU:HD23	1:C:188:VAL:CG2	2.44	0.42
1:B:282:ASN:OD1	1:B:310:GLU:HG2	2.19	0.42
1:F:61:ILE:CG1	1:F:112:VAL:HG22	2.49	0.42
1:F:217:LYS:NZ	2:F:430:HOH:O	2.43	0.42
1:F:238:LEU:N	1:F:238:LEU:HD23	2.34	0.42
1:F:261:GLU:HG2	1:F:308:ARG:HE	1.84	0.42
1:B:249:ILE:HG22	1:B:250:PHE:N	2.34	0.42
1:E:5:GLU:O	1:E:6:ASP:O	2.36	0.42
1:E:364:GLN:CD	1:E:364:GLN:H	2.26	0.42
1:F:319:ILE:N	1:F:319:ILE:HD12	2.34	0.42
1:A:195:ILE:C	1:A:197:GLN:H	2.26	0.42
1:A:195:ILE:C	1:A:197:GLN:N	2.77	0.42
1:A:217:PHE:HZ	1:A:244:LEU:HD13	1.84	0.42
1:A:358:VAL:C	1:A:360:GLN:H	2.27	0.42
1:A:362:GLU:HG2	1:C:90:ARG:CZ	2.49	0.42
1:B:9:ASN:C	1:B:9:ASN:ND2	2.77	0.42
1:B:101:GLN:CD	1:B:216:PRO:HD3	2.44	0.42
1:B:250:PHE:C	1:B:250:PHE:HD2	2.26	0.42
1:C:330:THR:O	1:C:331:SER:HB3	2.19	0.42
1:D:270:ALA:H	1:D:345:ASN:ND2	2.18	0.42
1:F:65:HIS:HA	1:F:138:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:ARG:HD3	1:F:213:ILE:CD1	2.49	0.42
1:F:205:ASN:C	1:F:207:PHE:H	2.28	0.42
1:F:235:GLU:HB2	1:F:332:ASN:N	2.34	0.42
1:A:23:PHE:CE2	1:A:186:VAL:HG22	2.55	0.42
1:B:382:LYS:HG3	1:B:382:LYS:O	2.18	0.42
1:E:37:ASN:N	1:E:37:ASN:ND2	2.56	0.42
1:F:71:PHE:CE2	1:F:126:ALA:HB2	2.55	0.42
1:F:80:ALA:HB2	1:F:120:LEU:CD2	2.49	0.42
1:A:351:ALA:N	1:A:356:ASN:OD1	2.52	0.42
1:B:269:LYS:H	1:B:345:ASN:ND2	2.16	0.42
1:C:71:PHE:HB2	1:C:103:ILE:HB	2.02	0.42
1:C:384:GLN:HE22	1:C:386:GLU:HB2	1.75	0.42
1:E:173:LEU:HA	1:F:370:PHE:HB3	2.02	0.42
1:E:305:GLN:NE2	2:E:432:HOH:O	2.52	0.42
1:F:170:ASN:ND2	1:F:170:ASN:C	2.75	0.42
1:A:302:LEU:HG	1:C:23:PHE:CZ	2.54	0.42
1:C:102:ARG:N	1:C:220:GLN:HE21	2.16	0.42
1:D:25:ASN:HB3	1:D:27:ASN:H	1.84	0.42
1:C:13:PHE:CZ	1:C:39:ARG:HG3	2.53	0.42
1:C:32:LEU:CD1	1:C:50:ARG:NH2	2.82	0.42
1:C:35:ARG:HG3	1:C:50:ARG:HE	1.84	0.42
1:D:71:PHE:HA	1:D:125:LEU:O	2.20	0.42
1:D:138:PHE:HB3	1:D:149:TYR:CD2	2.55	0.42
1:D:373:SER:O	1:D:374:ALA:C	2.61	0.42
1:F:31:ARG:HH21	1:F:53:GLN:NE2	2.18	0.42
1:F:37:ASN:ND2	1:F:38:LYS:H	2.17	0.42
1:F:38:LYS:HA	1:F:38:LYS:HD3	1.92	0.42
1:A:364:GLN:O	1:A:368:LEU:CD1	2.68	0.42
1:C:203:TYR:HB3	1:C:388:TYR:CD1	2.55	0.42
1:C:254:ASN:HB3	1:C:334:ASN:ND2	2.31	0.42
1:D:302:LEU:N	1:D:302:LEU:HD22	2.34	0.42
1:A:284:GLU:HB2	1:A:326:VAL:HG12	2.01	0.42
1:C:35:ARG:HG3	1:C:50:ARG:HH11	1.84	0.42
1:E:194:GLN:NE2	1:F:368:LEU:HD11	2.35	0.42
1:A:53:GLN:HE22	1:A:314:ASP:CG	2.26	0.41
1:A:248:ASP:OD2	1:A:343:GLU:HB2	2.20	0.41
1:A:278:GLU:HG2	1:A:279:GLY:N	2.35	0.41
1:A:364:GLN:H	1:A:364:GLN:HE21	1.57	0.41
1:B:6:ASP:HB2	1:B:12:TYR:CE1	2.55	0.41
1:B:35:ARG:NE	2:B:425:HOH:O	2.50	0.41
1:B:193:GLU:O	1:B:197:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ILE:HG21	1:D:302:LEU:CD1	2.48	0.41
1:E:205:SER:HA	1:E:209:THR:HG21	2.02	0.41
1:F:239:LEU:HD13	1:F:389:PHE:CE1	2.55	0.41
1:A:53:GLN:HE22	1:A:314:ASP:CB	2.33	0.41
1:B:87:ASN:ND2	1:B:88:ASP:N	2.65	0.41
1:C:77:SER:OG	1:C:121:LYS:HB3	2.19	0.41
1:D:212:SER:O	1:D:242:PRO:HG2	2.20	0.41
1:D:223:ASN:N	1:D:223:ASN:ND2	2.68	0.41
1:D:368:LEU:HD21	1:F:190:LEU:HA	2.02	0.41
1:E:83:THR:HG21	1:E:110:TYR:CE2	2.54	0.41
1:E:259:GLY:C	1:E:392:ALA:HB3	2.45	0.41
1:E:263:LEU:HD21	1:E:390:VAL:HG11	2.03	0.41
1:A:67:ALA:C	1:A:69:ALA:N	2.79	0.41
1:A:89:ASP:HA	1:B:360:GLN:NE2	2.35	0.41
1:A:171:ARG:O	1:A:181:ARG:NH2	2.48	0.41
1:A:331:SER:O	1:A:332:ASN:C	2.61	0.41
1:B:23:PHE:HA	2:B:452:HOH:O	2.18	0.41
1:B:148:SER:C	1:B:150:LEU:H	2.27	0.41
1:C:359:ARG:NH1	1:C:359:ARG:HB3	2.35	0.41
1:E:281:ALA:HB2	1:E:333:LEU:HD22	2.02	0.41
1:E:285:LEU:HB3	1:E:307:TYR:HB2	2.02	0.41
1:E:304:VAL:O	1:E:304:VAL:HG23	2.20	0.41
1:F:72:LEU:HB3	1:F:125:LEU:HB3	2.02	0.41
1:F:212:GLU:HA	1:F:228:LEU:O	2.21	0.41
1:A:364:GLN:NE2	1:A:364:GLN:N	2.54	0.41
1:C:40:SER:C	1:C:42:GLN:H	2.28	0.41
1:C:194:PHE:CD1	1:C:194:PHE:N	2.88	0.41
1:D:101:GLN:OE1	1:D:216:PRO:HD3	2.20	0.41
1:D:391:ASP:O	1:F:160:THR:CG2	2.69	0.41
1:E:219:LEU:CB	1:E:236:ILE:HG12	2.50	0.41
1:E:289:LYS:N	1:E:303:GLU:O	2.44	0.41
1:E:349:PHE:O	1:E:356:ASN:HA	2.20	0.41
1:F:214:THR:HB	1:F:215:PRO:CD	2.51	0.41
1:F:239:LEU:O	1:F:326:VAL:HG23	2.21	0.41
1:A:57:LYS:HB3	1:A:58:PRO:HD2	2.02	0.41
1:A:265:HIS:O	1:A:324:PRO:HA	2.21	0.41
1:B:83:THR:HB	1:B:92:SER:OG	2.20	0.41
1:E:306:ARG:HD2	1:E:308:ARG:NH2	2.36	0.41
1:F:197:ARG:NH2	1:F:232:ASP:OD2	2.53	0.41
1:A:59:ASN:HD22	1:A:195:ILE:CD1	2.33	0.41
1:A:141:SER:HB2	1:B:369:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:SER:C	1:B:150:LEU:N	2.78	0.41
1:B:384:GLN:HE21	1:B:386:GLU:H	1.69	0.41
1:C:260:ILE:CD1	1:C:311:LEU:HD11	2.47	0.41
1:D:151:GLN:OE1	1:D:176:GLU:OE1	2.37	0.41
1:D:363:ARG:NH1	1:D:374:ALA:HB3	2.35	0.41
1:E:220:ARG:C	1:E:222:ARG:H	2.29	0.41
1:F:246:LYS:H	1:F:345:ASN:ND2	2.16	0.41
1:A:45:ASN:ND2	1:C:129:VAL:O	2.52	0.41
1:B:194:GLN:O	1:B:198:LEU:HG	2.20	0.41
1:C:87:ASN:C	1:C:87:ASN:HD22	2.28	0.41
1:D:85:VAL:HG22	1:E:357:VAL:HG23	2.03	0.41
1:D:210:ILE:CD1	1:D:236:ILE:HD12	2.47	0.41
1:D:278:GLU:HG2	1:D:279:GLY:N	2.36	0.41
1:D:279:GLY:HA3	1:D:332:ASN:O	2.21	0.41
1:E:215:GLU:HB3	1:E:216:PRO:HD2	2.03	0.41
1:E:277:ASN:HB3	1:E:334:ASN:O	2.21	0.41
1:C:65:HIS:HB3	1:C:139:PHE:CD2	2.55	0.41
1:C:68:ASP:OD2	1:C:135:TYR:HB2	2.20	0.41
1:D:195:ILE:O	1:D:196:ARG:C	2.63	0.41
1:A:210:ILE:CD1	1:A:236:ILE:HD12	2.51	0.41
1:A:274:LEU:C	1:A:274:LEU:CD1	2.92	0.41
1:A:362:GLU:O	1:A:363:ARG:C	2.64	0.41
1:A:363:ARG:NH2	1:A:374:ALA:HB1	2.36	0.41
1:C:32:LEU:CD2	1:C:52:VAL:HG22	2.43	0.41
1:C:37:ASN:HD22	1:C:37:ASN:H	1.69	0.41
1:C:102:ARG:HB3	1:C:220:GLN:HE21	1.85	0.41
1:C:174:PHE:N	1:C:174:PHE:CD2	2.87	0.41
1:C:384:GLN:HE21	1:C:386:GLU:HB2	1.79	0.41
1:D:61:ILE:O	1:D:61:ILE:HG23	2.21	0.41
1:D:207:ARG:NH1	1:D:207:ARG:CG	2.82	0.41
1:E:6:ASP:C	1:E:8:ASN:N	2.78	0.41
1:E:82:LEU:O	1:E:93:TYR:N	2.49	0.41
1:E:83:THR:HA	1:E:92:SER:HA	2.03	0.41
1:E:238:PRO:HG3	1:E:249:ILE:O	2.21	0.41
1:F:195:ASN:HD22	1:F:198:SER:HB2	1.86	0.41
1:F:382:LYS:HA	1:F:382:LYS:HD2	1.89	0.41
1:A:13:PHE:HB2	1:A:316:VAL:O	2.20	0.41
1:B:90:ARG:NH2	1:B:201:ARG:NH1	2.69	0.41
1:B:319:ILE:HG21	1:B:325:PHE:CD1	2.56	0.41
1:C:24:GLU:HG3	1:C:29:ARG:HG3	2.01	0.41
1:D:80:ALA:HB2	1:D:120:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:PHE:CE2	1:D:186:VAL:HB	2.56	0.41
1:D:146:GLN:HB3	1:E:302:LEU:HB2	2.03	0.41
1:D:261:LEU:HD23	1:D:390:VAL:O	2.20	0.41
1:E:31:ARG:NH2	1:E:53:GLN:HE22	2.14	0.41
1:E:83:THR:HA	1:E:91:ASP:O	2.20	0.41
1:A:68:ASP:OD2	1:A:130:ASN:ND2	2.47	0.40
1:A:380:LEU:HD21	1:C:169:ILE:HG22	2.03	0.40
1:D:29:ARG:HG2	1:D:30:ILE:N	2.36	0.40
1:D:171:ARG:O	1:D:181:ARG:NH2	2.54	0.40
1:D:213:GLU:HA	1:D:242:PRO:HG2	2.03	0.40
1:E:343:GLU:O	1:E:344:ASN:HB2	2.21	0.40
1:F:59:ASN:OD1	1:F:116:ASP:HA	2.20	0.40
1:D:23:PHE:CE1	1:D:25:ASN:ND2	2.89	0.40
1:D:152:GLY:O	1:E:306:ARG:HG2	2.21	0.40
1:E:219:LEU:HB2	1:E:236:ILE:CD1	2.51	0.40
1:F:384:GLN:HE21	1:F:386:GLU:N	2.11	0.40
1:F:384:GLN:NE2	1:F:386:GLU:CB	2.84	0.40
1:A:54:PHE:CD2	1:A:122:MET:HE3	2.57	0.40
1:B:90:ARG:NH1	1:C:362:GLU:HG2	2.35	0.40
1:C:32:LEU:CD1	1:C:50:ARG:HH12	2.34	0.40
1:C:207:PHE:HB3	1:C:237:ALA:HB2	2.02	0.40
1:D:5:GLU:O	1:D:6:ASP:C	2.64	0.40
1:E:6:ASP:HB3	1:E:12:TYR:CD1	2.56	0.40
1:B:75:VAL:HA	1:B:122:MET:HG2	2.03	0.40
1:B:321:ALA:O	1:B:322:ALA:HB3	2.20	0.40
1:D:57:LYS:HB3	1:D:58:PRO:CD	2.50	0.40
1:D:101:GLN:HG3	1:D:102:ARG:N	2.36	0.40
1:E:101:GLN:CD	1:E:216:PRO:HD3	2.46	0.40
1:E:267:ASN:HB3	1:E:345:ASN:HD21	1.87	0.40
1:F:6:ASP:O	1:F:7:GLU:C	2.64	0.40
1:F:238:LEU:HD21	1:F:390:VAL:CG2	2.52	0.40
1:C:190:LEU:O	1:C:190:LEU:CD2	2.69	0.40
1:C:306:ARG:HG3	1:C:306:ARG:HH11	1.87	0.40
1:E:218:ASN:HD22	1:E:218:ASN:C	2.29	0.40
1:F:196:LEU:HD23	1:F:230:SER:HB2	2.04	0.40
1:F:258:ALA:CB	1:F:333:LEU:HD22	2.49	0.40
1:F:380:LEU:C	1:F:382:LYS:N	2.78	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	373/416 (90%)	348 (93%)	21 (6%)	4 (1%)	11	22
1	B	364/416 (88%)	343 (94%)	14 (4%)	7 (2%)	6	11
1	C	338/416 (81%)	306 (90%)	25 (7%)	7 (2%)	5	9
1	D	373/416 (90%)	342 (92%)	27 (7%)	4 (1%)	11	22
1	E	364/416 (88%)	340 (93%)	20 (6%)	4 (1%)	11	22
1	F	338/416 (81%)	295 (87%)	37 (11%)	6 (2%)	6	12
All	All	2150/2496 (86%)	1974 (92%)	144 (7%)	32 (2%)	8	16

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	ASP
1	C	7	GLU
1	D	6	ASP
1	E	6	ASP
1	E	201	ARG
1	F	7	GLU
1	F	331	SER
1	A	6	ASP
1	A	39	ARG
1	A	372	GLY
1	B	7	GLU
1	B	185	GLY
1	B	207	ARG
1	C	16	SER
1	C	184	GLU
1	B	388	TYR
1	D	39	ARG
1	D	372	GLY
1	F	206	ASN
1	B	229	ASN

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Mol	Chain	Res	Type
1	B	332	ASN
1	C	331	SER
1	F	15	SER
1	F	381	LEU
1	A	68	ASP
1	C	10	PRO
1	C	88	ASP
1	C	141	SER
1	D	68	ASP
1	E	39	ARG
1	E	388	TYR
1	F	10	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	341/375 (91%)	310 (91%)	31 (9%)	9	19
1	B	334/375 (89%)	303 (91%)	31 (9%)	8	18
1	C	311/375 (83%)	288 (93%)	23 (7%)	13	27
1	D	341/375 (91%)	309 (91%)	32 (9%)	8	18
1	E	334/375 (89%)	309 (92%)	25 (8%)	12	26
1	F	311/375 (83%)	286 (92%)	25 (8%)	11	24
All	All	1972/2250 (88%)	1805 (92%)	167 (8%)	10	22

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	22	LEU
1	A	26	GLN
1	A	29	ARG
1	A	32	LEU
1	A	37	ASN

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Mol	Chain	Res	Type
1	A	38	LYS
1	A	62	LEU
1	A	73	LEU
1	A	85	VAL
1	A	87	ASN
1	A	102	ARG
1	A	140	LEU
1	A	142	SER
1	A	146	GLN
1	A	151	GLN
1	A	157	ILE
1	A	160	THR
1	A	188	VAL
1	A	244	LEU
1	A	250	PHE
1	A	252	SER
1	A	254	VAL
1	A	274	LEU
1	A	275	VAL
1	A	278	GLU
1	A	285	LEU
1	A	318	VAL
1	A	359	ARG
1	A	360	GLN
1	A	364	GLN
1	B	22	LEU
1	B	26	GLN
1	B	37	ASN
1	B	39	ARG
1	B	53	GLN
1	B	62	LEU
1	B	83	THR
1	B	85	VAL
1	B	87	ASN
1	B	131	LYS
1	B	140	LEU
1	B	146	GLN
1	B	167	GLU
1	B	190	LEU
1	B	201	ARG
1	B	207	ARG
1	B	218	ASN

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Mol	Chain	Res	Type
1	B	239	GLU
1	B	244	LEU
1	B	250	PHE
1	B	254	VAL
1	B	257	ASN
1	B	261	LEU
1	B	274	LEU
1	B	275	VAL
1	B	286	VAL
1	B	318	VAL
1	B	346	GLN
1	B	359	ARG
1	B	368	LEU
1	B	380	LEU
1	C	8	ASN
1	C	22	LEU
1	C	25	ASN
1	C	39	ARG
1	C	40	SER
1	C	50	ARG
1	C	62	LEU
1	C	87	ASN
1	C	121	LYS
1	C	146	GLN
1	C	189	GLU
1	C	216	GLU
1	C	221	LEU
1	C	227	PHE
1	C	231	VAL
1	C	251	LEU
1	C	257	ASP
1	C	262	LEU
1	C	308	ARG
1	C	318	VAL
1	C	346	GLN
1	C	368	LEU
1	C	386	GLU
1	D	9	ASN
1	D	17	ASN
1	D	20	GLN
1	D	21	THR
1	D	22	LEU

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Mol	Chain	Res	Type
1	D	26	GLN
1	D	32	LEU
1	D	37	ASN
1	D	38	LYS
1	D	53	GLN
1	D	62	LEU
1	D	85	VAL
1	D	87	ASN
1	D	95	LEU
1	D	140	LEU
1	D	146	GLN
1	D	151	GLN
1	D	157	ILE
1	D	176	GLU
1	D	188	VAL
1	D	200	ARG
1	D	221	SER
1	D	244	LEU
1	D	254	VAL
1	D	258	GLU
1	D	274	LEU
1	D	275	VAL
1	D	285	LEU
1	D	318	VAL
1	D	360	GLN
1	D	380	LEU
1	D	385	ARG
1	E	6	ASP
1	E	8	ASN
1	E	9	ASN
1	E	20	GLN
1	E	22	LEU
1	E	26	GLN
1	E	37	ASN
1	E	62	LEU
1	E	83	THR
1	E	87	ASN
1	E	146	GLN
1	E	190	LEU
1	E	197	GLN
1	E	207	ARG
1	E	209	THR

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Mol	Chain	Res	Type
1	E	218	ASN
1	E	223	ASN
1	E	244	LEU
1	E	254	VAL
1	E	274	LEU
1	E	286	VAL
1	E	318	VAL
1	E	346	GLN
1	E	380	LEU
1	E	385	ARG
1	F	8	ASN
1	F	9	ASN
1	F	20	GLN
1	F	22	LEU
1	F	32	LEU
1	F	37	ASN
1	F	39	ARG
1	F	53	GLN
1	F	62	LEU
1	F	85	VAL
1	F	87	ASN
1	F	140	LEU
1	F	146	GLN
1	F	216	GLU
1	F	221	LEU
1	F	227	PHE
1	F	231	VAL
1	F	234	ASN
1	F	251	LEU
1	F	252	VAL
1	F	262	LEU
1	F	308	ARG
1	F	343	GLU
1	F	353	GLU
1	F	386	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (185) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	ASN
1	A	20	GLN

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Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	ASN
1	A	34	GLN
1	A	37	ASN
1	A	53	GLN
1	A	59	ASN
1	A	87	ASN
1	A	94	ASN
1	A	117	HIS
1	A	118	GLN
1	A	119	ASN
1	A	144	GLN
1	A	151	GLN
1	A	170	ASN
1	A	218	ASN
1	A	223	ASN
1	A	243	GLN
1	A	257	ASN
1	A	277	ASN
1	A	282	ASN
1	A	328	ASN
1	A	332	ASN
1	A	334	ASN
1	A	341	ASN
1	A	344	ASN
1	A	345	ASN
1	A	348	ASN
1	A	356	ASN
1	A	360	GLN
1	A	364	GLN
1	A	384	GLN
1	B	8	ASN
1	B	9	ASN
1	B	26	GLN
1	B	27	ASN
1	B	34	GLN
1	B	37	ASN
1	B	53	GLN
1	B	59	ASN
1	B	87	ASN
1	B	94	ASN
1	B	118	GLN

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Mol	Chain	Res	Type
1	B	119	ASN
1	B	144	GLN
1	B	146	GLN
1	B	147	GLN
1	B	151	GLN
1	B	218	ASN
1	B	229	ASN
1	B	243	GLN
1	B	257	ASN
1	B	277	ASN
1	B	328	ASN
1	B	332	ASN
1	B	334	ASN
1	B	341	ASN
1	B	345	ASN
1	B	346	GLN
1	B	360	GLN
1	B	384	GLN
1	C	8	ASN
1	C	9	ASN
1	C	37	ASN
1	C	45	ASN
1	C	53	GLN
1	C	59	ASN
1	C	65	HIS
1	C	87	ASN
1	C	94	ASN
1	C	113	ASN
1	C	118	GLN
1	C	119	ASN
1	C	146	GLN
1	C	155	HIS
1	C	156	ASN
1	C	170	ASN
1	C	183	GLN
1	C	220	GLN
1	C	234	ASN
1	C	254	ASN
1	C	259	ASN
1	C	328	ASN
1	C	332	ASN
1	C	334	ASN

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Mol	Chain	Res	Type
1	C	341	ASN
1	C	345	ASN
1	C	346	GLN
1	C	348	ASN
1	C	360	GLN
1	C	384	GLN
1	D	8	ASN
1	D	9	ASN
1	D	17	ASN
1	D	20	GLN
1	D	25	ASN
1	D	26	GLN
1	D	27	ASN
1	D	34	GLN
1	D	37	ASN
1	D	53	GLN
1	D	59	ASN
1	D	87	ASN
1	D	94	ASN
1	D	119	ASN
1	D	144	GLN
1	D	151	GLN
1	D	170	ASN
1	D	194	GLN
1	D	218	ASN
1	D	223	ASN
1	D	243	GLN
1	D	257	ASN
1	D	277	ASN
1	D	282	ASN
1	D	332	ASN
1	D	334	ASN
1	D	341	ASN
1	D	344	ASN
1	D	345	ASN
1	D	348	ASN
1	D	356	ASN
1	D	360	GLN
1	D	384	GLN
1	E	8	ASN
1	E	9	ASN
1	E	26	GLN

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Mol	Chain	Res	Type
1	E	27	ASN
1	E	34	GLN
1	E	37	ASN
1	E	45	ASN
1	E	53	GLN
1	E	59	ASN
1	E	87	ASN
1	E	94	ASN
1	E	118	GLN
1	E	119	ASN
1	E	144	GLN
1	E	146	GLN
1	E	147	GLN
1	E	151	GLN
1	E	194	GLN
1	E	218	ASN
1	E	229	ASN
1	E	243	GLN
1	E	257	ASN
1	E	277	ASN
1	E	305	GLN
1	E	328	ASN
1	E	332	ASN
1	E	334	ASN
1	E	341	ASN
1	E	345	ASN
1	E	360	GLN
1	E	384	GLN
1	F	8	ASN
1	F	9	ASN
1	F	34	GLN
1	F	37	ASN
1	F	45	ASN
1	F	53	GLN
1	F	87	ASN
1	F	94	ASN
1	F	117	HIS
1	F	118	GLN
1	F	119	ASN
1	F	146	GLN
1	F	147	GLN
1	F	170	ASN

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Mol	Chain	Res	Type
1	F	195	ASN
1	F	218	ASN
1	F	220	GLN
1	F	234	ASN
1	F	242	HIS
1	F	254	ASN
1	F	305	GLN
1	F	328	ASN
1	F	332	ASN
1	F	334	ASN
1	F	341	ASN
1	F	345	ASN
1	F	348	ASN
1	F	384	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	377/416 (90%)	-0.66	0 100 100	18, 34, 67, 82	0
1	B	370/416 (88%)	-0.57	2 (0%) 87 85	14, 36, 62, 76	0
1	C	346/416 (83%)	-0.21	1 (0%) 90 87	25, 54, 74, 85	0
1	D	377/416 (90%)	-0.65	0 100 100	17, 32, 67, 80	0
1	E	370/416 (88%)	-0.55	0 100 100	15, 39, 69, 78	0
1	F	346/416 (83%)	-0.26	1 (0%) 90 87	28, 53, 75, 84	0
All	All	2186/2496 (87%)	-0.49	4 (0%) 91 89	14, 40, 70, 85	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	ASN	2.5
1	B	392	ALA	2.2
1	F	392	ALA	2.1
1	C	89	ASP	2.1

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.