



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:51 AM UTC

PDB ID : 3JUA / pdb_00003jua
Title : Structural basis of YAP recognition by TEAD4 in the Hippo pathway
Authors : Chen, L.; Song, H.
Deposited on : 2009-09-15
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

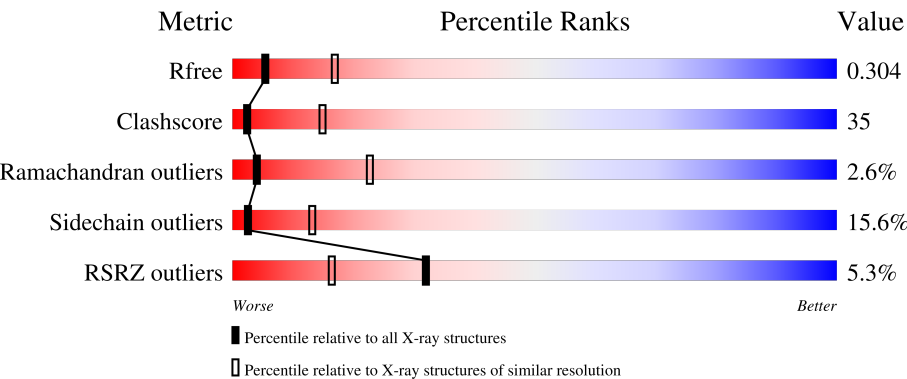
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	220	45% 40% 6% 7%
1	C	220	4% 55% 31% 9%
1	E	220	4% 49% 35% 12%
1	G	220	6% 47% 28% 9% 14%
2	B	39	8% 21% 59% 18%

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Mol	Chain	Length	Quality of chain
2	D	39	5% 46% 28% 13% • 10%
2	F	39	26% 31% 51% 5% 5% 8%
2	H	39	8% 18% 10% 18% • 51%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8055 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 Transcriptional enhancer factor TEF-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1692	1092	281	309	10			
1	C	213	Total	C	N	O	S	0	0	0
			1762	1131	293	328	10			
1	E	216	Total	C	N	O	S	0	0	0
			1782	1144	294	334	10			
1	G	190	Total	C	N	O	S	0	0	0
			1586	1021	263	292	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	SER	-	expression tag	UNP Q62296
A	209	MET	-	expression tag	UNP Q62296
C	208	SER	-	expression tag	UNP Q62296
C	209	MET	-	expression tag	UNP Q62296
E	208	SER	-	expression tag	UNP Q62296
E	209	MET	-	expression tag	UNP Q62296
G	208	SER	-	expression tag	UNP Q62296
G	209	MET	-	expression tag	UNP Q62296

- Molecule 2 is a protein called 65 kDa Yes-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	S	0	0	0
			311	200	52	57	2			
2	D	35	Total	C	N	O	S	0	0	0
			279	180	48	49	2			
2	F	36	Total	C	N	O	S	0	0	0
			286	185	49	50	2			
2	H	19	Total	C	N	O	S	0	0	0
			158	105	28	24	1			

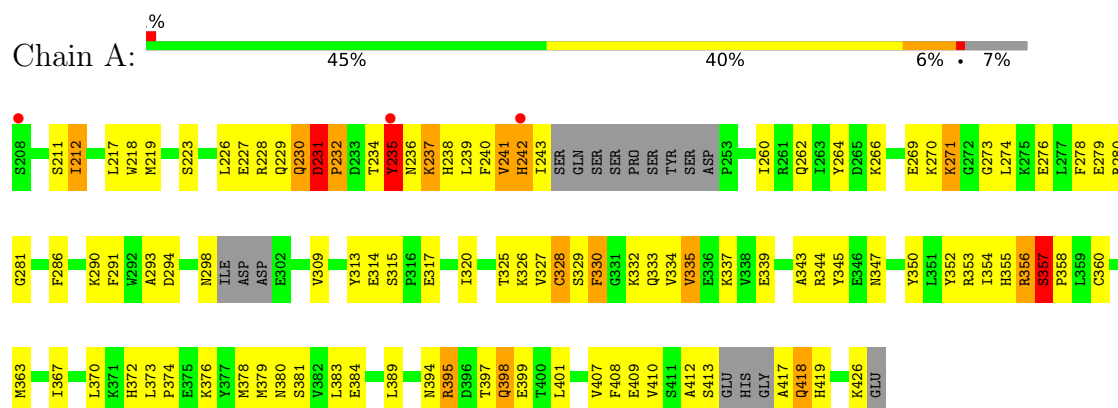
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	7	Total O 7 7	0	0
3	C	45	Total O 45 45	0	0
3	D	6	Total O 6 6	0	0
3	E	51	Total O 51 51	0	0
3	F	7	Total O 7 7	0	0
3	G	42	Total O 42 42	0	0

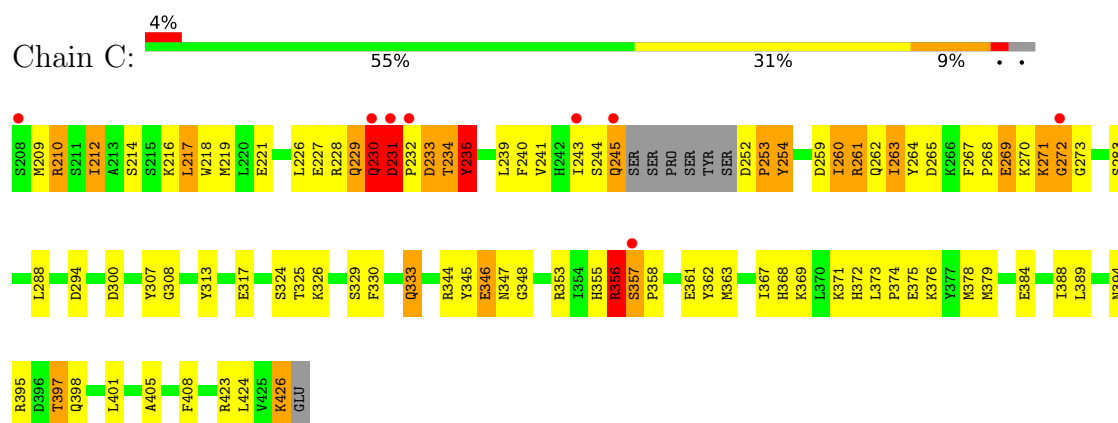
3 Residue-property plots [i](#)

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

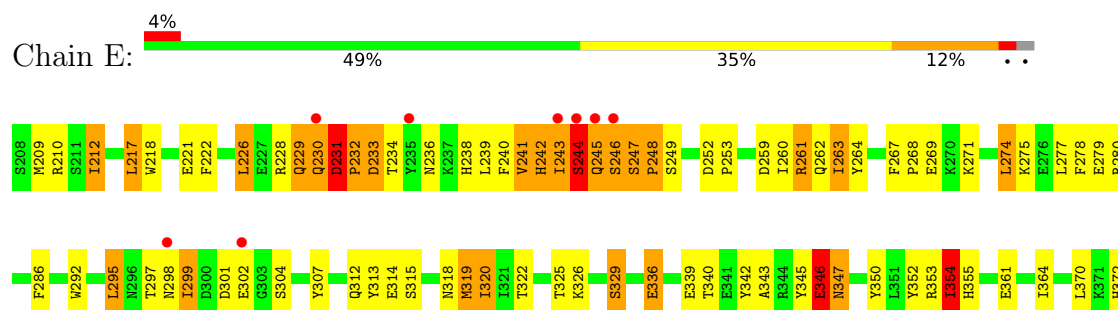
• Molecule 1: Transcriptional enhancer factor TEF-3

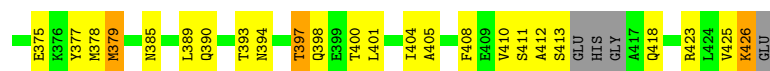


• Molecule 1: Transcriptional enhancer factor TEF-3

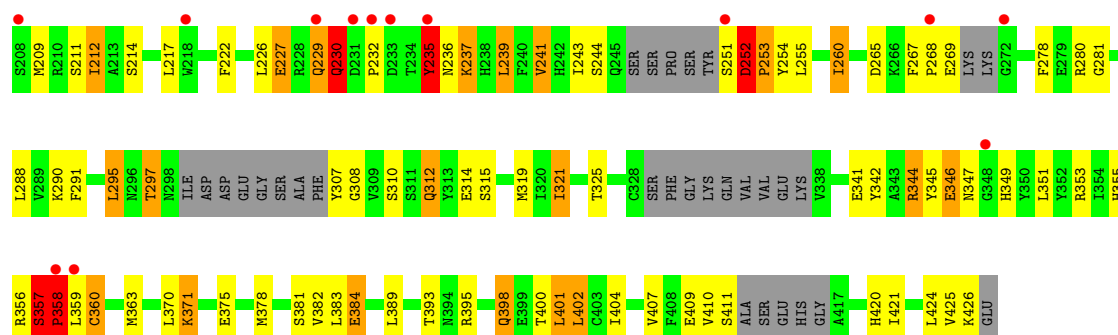


• Molecule 1: Transcriptional enhancer factor TEF-3

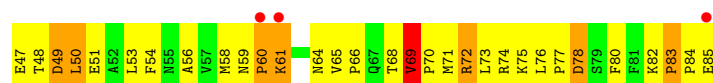




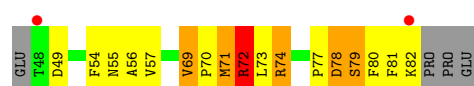
- Molecule 1: Transcriptional enhancer factor TEF-3



- Molecule 2: 65 kDa Yes-associated protein



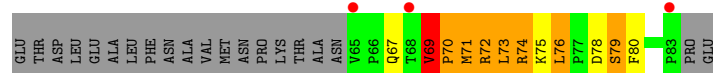
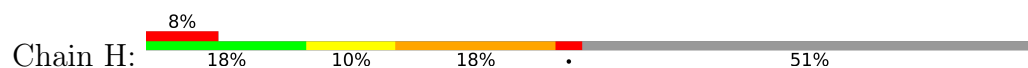
- Molecule 2: 65 kDa Yes-associated protein



- Molecule 2: 65 kDa Yes-associated protein



- Molecule 2: 65 kDa Yes-associated protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.98Å 146.91Å 165.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.00) 99.5 (20.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.236 , 0.288 0.255 , 0.304	Depositor DCC
R_{free} test set	3103 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8055	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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	0.69	0/1733	0.97	3/2335 (0.1%)
1	C	0.75	0/1806	1.27	20/2438 (0.8%)
1	E	0.76	2/1827 (0.1%)	1.21	14/2468 (0.6%)
1	G	0.62	1/1623 (0.1%)	1.21	11/2189 (0.5%)
2	B	0.64	0/319	1.13	6/434 (1.4%)
2	D	0.86	1/285 (0.4%)	1.34	2/386 (0.5%)
2	F	0.93	1/293 (0.3%)	1.30	4/398 (1.0%)
2	H	0.65	0/163	1.62	5/220 (2.3%)
All	All	0.72	5/8049 (0.1%)	1.19	65/10868 (0.6%)

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	A	0	1
1	C	0	3
1	E	0	1
1	G	0	1
2	F	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	72	ARG	CA-C	-6.13	1.47	1.53
2	D	72	ARG	N-CA	-5.44	1.40	1.46
1	E	354	ILE	CA-CB	-5.33	1.47	1.54
1	E	248	PRO	CA-C	-5.19	1.46	1.52
1	G	357	SER	CA-C	-5.07	1.46	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	357	SER	C-N-CD	-19.15	78.46	120.60
1	G	346	GLU	N-CA-C	-15.99	86.74	109.29
1	E	248	PRO	N-CA-C	-14.14	91.11	111.33
1	G	230	GLN	N-CA-C	-12.68	83.78	110.80
2	H	72	ARG	N-CA-C	-12.07	95.56	110.41
1	C	253	PRO	N-CA-C	-12.06	94.09	111.33
1	C	231	ASP	N-CA-C	-11.11	96.82	109.60
1	G	357	SER	N-CA-C	11.03	134.18	109.81
1	E	247	SER	N-CA-C	-10.39	86.84	109.81
1	C	230	GLN	N-CA-C	-10.34	92.95	109.59
1	C	272	GLY	N-CA-C	-10.16	89.10	113.18
1	C	254	TYR	N-CA-C	-10.06	93.60	109.50
1	G	358	PRO	N-CA-C	-9.87	86.45	112.10
1	G	252	ASP	C-N-CD	-9.66	85.37	125.00
1	E	210	ARG	N-CA-C	-9.26	102.12	113.41
1	C	233	ASP	N-CA-C	9.20	124.07	110.46
1	E	244	SER	N-CA-C	-8.82	92.02	110.80
1	G	235	TYR	N-CA-C	8.77	122.82	109.23
1	G	357	SER	CA-C-N	8.55	147.53	127.00
1	G	357	SER	C-N-CA	8.55	147.53	127.00
1	G	252	ASP	N-CA-C	8.48	128.56	109.81
2	D	72	ARG	N-CA-C	-8.44	99.80	112.54
1	A	235	TYR	N-CA-C	8.33	122.14	109.23
1	C	397	THR	N-CA-C	-8.06	99.89	110.53
2	H	69	VAL	CA-C-N	8.04	129.88	119.84
2	H	69	VAL	C-N-CA	8.04	129.88	119.84
1	C	346	GLU	CA-C-N	-7.81	113.15	122.44
1	C	346	GLU	C-N-CA	-7.81	113.15	122.44
2	F	64	ASN	N-CA-C	-7.78	94.41	108.02
1	C	348	GLY	N-CA-C	-7.67	95.00	113.18
2	H	71	MET	N-CA-C	7.25	119.81	111.11
2	B	69	VAL	N-CA-C	7.13	114.61	107.55
1	C	273	GLY	N-CA-C	-6.91	98.98	110.80
1	C	269	GLU	N-CA-C	6.82	123.60	114.12
1	C	235	TYR	N-CA-C	6.61	119.11	107.61
2	F	61	LYS	CB-CA-C	-6.53	98.47	112.12
2	D	71	MET	CB-CA-C	-6.37	98.28	110.57
2	F	72	ARG	N-CA-C	-6.37	100.73	109.71
1	E	269	GLU	CA-C-N	-6.31	114.93	122.44
1	E	269	GLU	C-N-CA	-6.31	114.93	122.44
2	B	64	ASN	N-CA-C	6.06	118.57	108.20
1	E	397	THR	N-CA-C	-5.94	102.16	110.35
1	E	269	GLU	N-CA-C	5.87	122.28	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	249	SER	N-CA-C	-5.69	100.08	108.79
2	B	83	PRO	N-CA-C	-5.56	103.92	110.70
1	C	231	ASP	C-N-CD	-5.56	108.37	120.60
1	E	231	ASP	C-N-CD	-5.55	108.39	120.60
1	C	397	THR	CA-C-N	-5.54	113.75	122.95
1	C	397	THR	C-N-CA	-5.54	113.75	122.95
2	F	73	LEU	CB-CA-C	-5.50	102.68	111.86
1	E	355	HIS	N-CA-C	5.39	117.53	107.99
1	G	359	LEU	N-CA-C	-5.34	105.46	111.28
1	C	270	LYS	N-CA-C	5.31	121.30	114.56
1	C	373	LEU	CA-C-N	5.28	126.44	119.84
1	C	373	LEU	C-N-CA	5.28	126.44	119.84
1	C	347	ASN	N-CA-C	5.26	119.02	111.02
2	B	69	VAL	CA-C-N	5.25	125.54	119.92
2	B	69	VAL	C-N-CA	5.25	125.54	119.92
1	E	408	PHE	N-CA-C	5.22	117.97	109.24
1	E	346	GLU	N-CA-C	-5.13	102.56	109.95
1	A	330	PHE	N-CA-C	-5.07	105.95	113.40
2	B	72	ARG	N-CA-C	-5.05	107.18	113.19
1	E	241	VAL	N-CA-C	-5.02	102.55	110.09
2	H	67	GLN	N-CA-C	5.02	121.48	110.80
1	A	358	PRO	N-CA-C	5.00	122.78	112.47

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	SER	Peptide
1	C	229	GLN	Peptide
1	C	231	ASP	Peptide
1	C	357	SER	Peptide
1	E	229	GLN	Peptide
2	F	72	ARG	Peptide
1	G	229	GLN	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	1692	0	1657	127	0
1	C	1762	0	1710	106	0
1	E	1782	0	1730	119	0
1	G	1586	0	1537	98	0
2	B	311	0	315	29	0
2	D	279	0	289	34	0
2	F	286	0	296	28	0
2	H	158	0	170	30	0
3	A	41	0	0	3	0
3	B	7	0	0	3	0
3	C	45	0	0	10	0
3	D	6	0	0	3	0
3	E	51	0	0	6	0
3	F	7	0	0	1	0
3	G	42	0	0	9	0
All	All	8055	0	7704	546	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 35.

All (546) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:69:VAL:HG12	2:H:70:PRO:CD	1.54	1.38
1:G:252:ASP:CB	1:G:253:PRO:HD3	1.30	1.37
2:H:75:LYS:O	2:H:76:LEU:HD23	1.18	1.32
1:C:210:ARG:HD3	1:C:252:ASP:OD1	1.27	1.25
2:H:75:LYS:C	2:H:76:LEU:HD23	1.62	1.24
1:C:271:LYS:HD2	1:C:271:LYS:C	1.33	1.24
1:C:271:LYS:CD	1:C:271:LYS:O	1.87	1.23
1:E:246:SER:C	1:E:248:PRO:HD3	1.62	1.23
1:C:210:ARG:CD	1:C:252:ASP:OD1	1.86	1.22
1:C:271:LYS:C	1:C:271:LYS:CD	2.04	1.22
1:C:271:LYS:HD2	1:C:271:LYS:O	0.99	1.16
2:H:72:ARG:C	2:H:73:LEU:HD23	1.69	1.15
1:C:261:ARG:HG3	1:C:261:ARG:HH11	1.04	1.15
1:G:308:GLY:HA2	1:G:358:PRO:HG3	1.22	1.13
1:G:252:ASP:CB	1:G:253:PRO:CD	2.26	1.12
1:G:252:ASP:HB3	1:G:253:PRO:HD3	1.26	1.11
1:C:235:TYR:N	1:E:232:PRO:HG2	1.65	1.11
1:E:243:ILE:O	1:E:245:GLN:N	1.85	1.10
1:E:230:GLN:O	1:E:232:PRO:HA	1.51	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LYS:HZ2	1:A:237:LYS:CA	1.62	1.09
2:F:73:LEU:HD23	2:F:73:LEU:O	1.52	1.08
2:H:73:LEU:N	2:H:73:LEU:CD2	2.15	1.07
1:C:210:ARG:HD3	1:C:252:ASP:CG	1.79	1.07
2:F:61:LYS:CG	2:F:61:LYS:O	1.98	1.06
2:H:73:LEU:HD23	2:H:73:LEU:N	1.68	1.06
1:C:232:PRO:HG3	3:C:168:HOH:O	1.54	1.06
1:G:280:ARG:O	1:G:280:ARG:HD3	1.56	1.05
2:H:75:LYS:O	2:H:76:LEU:CD2	2.04	1.05
2:F:73:LEU:HD22	2:F:73:LEU:N	1.62	1.04
1:G:229:GLN:HB3	1:G:230:GLN:O	1.57	1.04
1:C:245:GLN:OE1	1:C:245:GLN:HA	1.50	1.04
1:G:345:TYR:OH	1:G:347:ASN:O	1.73	1.03
2:F:73:LEU:HD22	2:F:73:LEU:H	0.87	1.03
1:G:358:PRO:HB2	3:G:177:HOH:O	1.57	1.03
1:C:227:GLU:HB3	1:C:235:TYR:HB2	1.04	1.03
1:C:235:TYR:H	1:E:232:PRO:HG2	0.87	1.02
1:G:252:ASP:HB2	1:G:253:PRO:HD3	1.40	1.02
1:G:237:LYS:NZ	1:G:237:LYS:HB3	1.74	1.01
1:A:230:GLN:O	1:A:232:PRO:HD2	1.60	1.00
2:H:69:VAL:CG1	2:H:70:PRO:CD	2.38	1.00
1:E:231:ASP:HB2	3:E:26:HOH:O	1.59	1.00
1:C:235:TYR:H	1:E:232:PRO:CG	1.73	1.00
1:A:237:LYS:CA	1:A:237:LYS:NZ	2.23	0.99
1:C:227:GLU:HB3	1:C:235:TYR:CB	1.91	0.99
1:A:270:LYS:C	1:A:271:LYS:HD2	1.88	0.99
2:H:69:VAL:CG1	2:H:70:PRO:HD2	1.92	0.99
1:A:270:LYS:O	1:A:271:LYS:HB2	1.64	0.98
2:F:73:LEU:HD23	2:F:73:LEU:C	1.87	0.98
1:A:237:LYS:NZ	1:A:237:LYS:HA	1.79	0.98
1:C:261:ARG:HH11	1:C:261:ARG:CG	1.76	0.98
1:A:426:LYS:HA	3:A:14:HOH:O	1.64	0.97
2:F:73:LEU:C	2:F:73:LEU:CD2	2.38	0.97
1:G:398:GLN:NE2	1:G:398:GLN:HA	1.79	0.97
2:F:73:LEU:H	2:F:73:LEU:CD2	1.75	0.96
1:G:345:TYR:CZ	1:G:347:ASN:O	2.18	0.95
1:C:227:GLU:CB	1:C:235:TYR:HB2	1.95	0.95
1:G:226:LEU:O	1:G:235:TYR:HB2	1.67	0.95
2:H:69:VAL:HG12	2:H:70:PRO:HD2	0.96	0.93
1:E:246:SER:OG	1:E:248:PRO:HD3	1.70	0.91
2:F:61:LYS:O	2:F:61:LYS:HG2	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:SER:C	1:E:248:PRO:CD	2.44	0.91
2:F:61:LYS:O	2:F:61:LYS:CD	2.19	0.91
1:G:260:ILE:HD11	1:G:426:LYS:HA	1.50	0.90
1:A:229:GLN:O	1:A:230:GLN:HG2	1.72	0.89
1:C:218:TRP:HE1	1:C:243:ILE:HG21	1.37	0.89
1:E:232:PRO:CB	1:E:233:ASP:HB2	2.02	0.89
2:F:61:LYS:O	2:F:61:LYS:HD3	1.71	0.88
1:G:310:SER:HB3	1:G:355:HIS:O	1.74	0.88
2:D:71:MET:CE	2:D:74:ARG:CZ	2.52	0.88
1:C:229:GLN:HB3	1:C:233:ASP:HB3	1.56	0.88
1:A:237:LYS:HZ2	1:A:237:LYS:N	1.71	0.88
1:C:261:ARG:HG3	1:C:261:ARG:NH1	1.84	0.87
1:E:240:PHE:HZ	1:E:243:ILE:HG23	1.39	0.87
1:G:345:TYR:CD1	1:G:346:GLU:O	2.27	0.87
2:H:72:ARG:HB2	2:H:73:LEU:HD23	1.55	0.87
1:A:329:SER:O	1:A:330:PHE:HB2	1.74	0.85
1:E:261:ARG:HG3	1:E:261:ARG:HH11	1.40	0.85
1:A:380:ASN:HD21	1:A:410:VAL:H	1.24	0.85
1:E:320:ILE:HD13	1:E:342:TYR:CE1	2.11	0.85
1:G:307:TYR:O	1:G:358:PRO:HG2	1.76	0.85
1:C:426:LYS:HB2	1:C:426:LYS:NZ	1.91	0.85
1:C:376:LYS:HA	1:C:379:MET:HE3	1.58	0.84
1:G:252:ASP:HB3	1:G:253:PRO:CD	1.98	0.84
1:G:237:LYS:HB3	1:G:237:LYS:HZ3	1.39	0.84
1:G:280:ARG:HD3	1:G:280:ARG:C	2.00	0.84
1:A:230:GLN:O	1:A:232:PRO:CD	2.26	0.84
1:E:240:PHE:HZ	1:E:243:ILE:CG2	1.90	0.84
1:A:229:GLN:O	1:A:230:GLN:CG	2.26	0.84
1:A:231:ASP:HB2	1:A:232:PRO:HD3	1.60	0.83
1:A:238:HIS:O	1:A:239:LEU:HG	1.77	0.83
1:C:210:ARG:CG	1:C:252:ASP:OD1	2.26	0.83
1:G:308:GLY:CA	1:G:358:PRO:HG3	2.08	0.83
1:E:261:ARG:HH11	1:E:261:ARG:CG	1.92	0.82
1:A:212:ILE:HG22	1:A:243:ILE:HD11	1.62	0.82
1:C:245:GLN:OE1	1:C:245:GLN:CA	2.29	0.81
1:G:229:GLN:CB	1:G:230:GLN:O	2.27	0.81
1:C:212:ILE:HG23	1:C:243:ILE:HD11	1.62	0.80
1:A:229:GLN:HG3	1:A:230:GLN:H	1.47	0.80
1:C:214:SER:OG	1:C:217:LEU:N	2.15	0.79
2:B:59:ASN:H	2:B:60:PRO:HA	1.48	0.79
1:E:354:ILE:O	1:E:354:ILE:HG22	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:80:PHE:O	2:H:80:PHE:CD1	2.36	0.78
2:H:72:ARG:CB	2:H:73:LEU:HD23	2.12	0.78
1:E:243:ILE:C	1:E:245:GLN:N	2.41	0.78
1:A:229:GLN:CG	1:A:230:GLN:H	1.97	0.78
1:A:237:LYS:NZ	1:A:237:LYS:N	2.32	0.78
1:E:246:SER:OG	1:E:248:PRO:HG3	1.83	0.77
1:E:325:THR:HG22	1:E:390:GLN:HG3	1.66	0.77
1:A:355:HIS:O	1:A:356:ARG:C	2.26	0.77
1:E:221:GLU:OE2	1:E:243:ILE:HG22	1.84	0.77
1:A:227:GLU:HB2	1:A:235:TYR:HB3	1.66	0.77
1:A:238:HIS:O	1:A:239:LEU:CD2	2.33	0.77
1:A:230:GLN:C	1:A:231:ASP:OD2	2.28	0.77
2:H:72:ARG:HB2	2:H:73:LEU:CD2	2.14	0.76
1:A:270:LYS:O	1:A:271:LYS:CB	2.33	0.76
2:H:69:VAL:CG1	2:H:70:PRO:HD3	2.16	0.76
1:E:246:SER:OG	1:E:248:PRO:CD	2.32	0.76
1:A:229:GLN:CG	1:A:230:GLN:N	2.48	0.76
1:E:240:PHE:CZ	1:E:243:ILE:HG23	2.21	0.76
1:C:426:LYS:HB2	1:C:426:LYS:HZ2	1.50	0.76
1:A:238:HIS:C	1:A:239:LEU:HG	2.10	0.75
1:C:271:LYS:CG	1:C:272:GLY:N	2.49	0.75
1:G:346:GLU:HG2	1:G:349:HIS:CE1	2.20	0.75
1:C:271:LYS:HG3	1:C:272:GLY:N	2.02	0.75
1:G:307:TYR:O	1:G:358:PRO:CG	2.35	0.75
1:A:227:GLU:CB	1:A:235:TYR:HB3	2.16	0.75
1:E:247:SER:C	1:E:248:PRO:O	2.16	0.75
2:D:71:MET:HA	2:D:74:ARG:HD3	1.69	0.75
1:G:212:ILE:HG22	1:G:243:ILE:HG13	1.69	0.75
2:F:73:LEU:O	2:F:73:LEU:CD2	2.30	0.75
1:A:238:HIS:O	1:A:239:LEU:CG	2.35	0.74
1:A:380:ASN:ND2	1:A:410:VAL:H	1.83	0.74
1:A:271:LYS:O	1:A:276:GLU:CD	2.30	0.73
1:C:374:PRO:HD2	1:C:378:MET:HE1	1.68	0.73
1:A:237:LYS:HA	1:A:237:LYS:HZ1	1.49	0.73
1:A:230:GLN:O	1:A:231:ASP:CG	2.31	0.73
2:H:70:PRO:O	2:H:72:ARG:O	2.06	0.73
1:C:271:LYS:HD2	1:C:272:GLY:N	2.01	0.73
1:E:209:MET:HE2	1:E:423:ARG:HE	1.54	0.73
1:E:232:PRO:HB3	1:E:233:ASP:HB2	1.70	0.73
1:A:334:VAL:HG23	1:A:335:VAL:HG12	1.70	0.72
1:E:246:SER:OG	1:E:248:PRO:CG	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:GLN:C	1:G:230:GLN:O	2.18	0.72
2:H:73:LEU:N	2:H:73:LEU:HD22	2.04	0.72
1:G:237:LYS:HB3	1:G:237:LYS:HZ2	1.55	0.71
1:G:400:THR:HG21	3:G:154:HOH:O	1.88	0.71
1:E:347:ASN:OD1	1:E:347:ASN:N	2.22	0.71
2:D:71:MET:CE	2:D:74:ARG:NE	2.54	0.70
1:E:260:ILE:HD11	1:E:274:LEU:HD22	1.74	0.70
1:A:226:LEU:O	1:A:235:TYR:HB2	1.92	0.70
2:D:71:MET:HA	2:D:71:MET:HE2	1.72	0.70
1:G:370:LEU:HD11	1:G:383:LEU:HD21	1.74	0.70
1:A:229:GLN:O	1:A:230:GLN:CB	2.39	0.70
2:D:69:VAL:O	2:D:74:ARG:NH1	2.25	0.70
1:E:246:SER:O	1:E:248:PRO:HD3	1.91	0.70
1:G:260:ILE:HG23	1:G:424:LEU:HB3	1.74	0.70
1:C:356:ARG:HD3	3:C:158:HOH:O	1.91	0.69
1:C:230:GLN:O	1:C:232:PRO:O	2.10	0.69
2:F:77:PRO:HD2	2:F:80:PHE:HB2	1.74	0.69
1:A:270:LYS:C	1:A:271:LYS:CD	2.66	0.69
1:A:337:LYS:HD3	3:A:144:HOH:O	1.94	0.68
1:A:356:ARG:C	1:A:357:SER:O	2.31	0.68
1:E:261:ARG:HG3	1:E:261:ARG:NH1	2.07	0.68
1:C:212:ILE:CG2	1:C:243:ILE:HD11	2.25	0.68
2:B:78:ASP:OD2	2:B:78:ASP:N	2.26	0.67
1:C:252:ASP:C	1:C:253:PRO:O	2.30	0.67
1:A:231:ASP:CB	1:A:232:PRO:HD3	2.23	0.67
1:C:210:ARG:HB3	1:C:252:ASP:OD1	1.95	0.67
1:E:412:ALA:O	1:E:413:SER:C	2.37	0.67
1:A:212:ILE:HD13	1:A:212:ILE:C	2.20	0.67
1:A:355:HIS:O	1:A:357:SER:N	2.28	0.66
1:C:234:THR:HA	1:E:232:PRO:HB2	1.78	0.66
2:D:71:MET:HE2	2:D:74:ARG:HD3	1.77	0.66
1:A:317:GLU:HG3	1:C:317:GLU:OE2	1.95	0.66
2:D:71:MET:O	2:D:81:PHE:HZ	1.78	0.66
1:E:297:THR:O	1:E:297:THR:HG23	1.95	0.66
1:G:360:CYS:SG	1:G:363:MET:HG2	2.36	0.66
2:B:59:ASN:N	2:B:60:PRO:HA	2.06	0.65
2:H:69:VAL:HG12	2:H:70:PRO:HD3	1.64	0.65
2:H:72:ARG:CA	2:H:73:LEU:HD23	2.26	0.65
1:C:267:PHE:HB3	1:C:268:PRO:HD2	1.78	0.65
1:G:243:ILE:HG22	1:G:244:SER:N	2.11	0.65
2:F:73:LEU:N	2:F:73:LEU:CD2	2.34	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HE3	2:B:71:MET:SD	2.37	0.64
2:D:72:ARG:HA	2:D:81:PHE:CZ	2.32	0.64
2:D:71:MET:HE3	2:D:74:ARG:CZ	2.27	0.64
1:A:397:THR:C	1:A:399:GLU:H	2.06	0.64
2:H:72:ARG:C	2:H:73:LEU:CD2	2.54	0.64
1:A:376:LYS:O	1:A:379:MET:HB2	1.98	0.64
1:C:230:GLN:O	1:C:231:ASP:C	2.41	0.64
1:G:357:SER:N	1:G:358:PRO:HD3	2.03	0.63
1:G:398:GLN:HA	1:G:398:GLN:HE21	1.56	0.63
1:A:229:GLN:HG2	1:A:230:GLN:N	2.14	0.63
1:C:356:ARG:O	1:C:356:ARG:HG3	1.97	0.63
1:C:229:GLN:HB3	1:C:233:ASP:CB	2.26	0.63
1:G:252:ASP:HB3	1:G:253:PRO:CG	2.29	0.63
1:C:356:ARG:CD	3:C:158:HOH:O	2.46	0.63
1:E:246:SER:CB	1:E:248:PRO:HD3	2.29	0.63
2:F:76:LEU:HB3	2:F:77:PRO:CD	2.28	0.63
2:B:48:THR:C	2:B:50:LEU:H	2.07	0.63
1:E:320:ILE:HD13	1:E:342:TYR:HE1	1.60	0.63
1:A:294:ASP:OD1	1:A:294:ASP:C	2.41	0.62
1:C:210:ARG:CB	1:C:252:ASP:OD1	2.47	0.62
1:C:212:ILE:HG12	1:C:212:ILE:O	1.97	0.62
1:A:239:LEU:HD21	1:A:293:ALA:HA	1.81	0.62
1:C:214:SER:HB3	1:C:401:LEU:O	2.00	0.62
1:G:229:GLN:CA	1:G:230:GLN:O	2.46	0.62
1:A:344:ARG:HD2	1:G:342:TYR:O	1.99	0.62
1:C:267:PHE:HB3	1:C:268:PRO:CD	2.28	0.62
1:C:271:LYS:CD	1:C:272:GLY:N	2.61	0.62
2:D:81:PHE:O	2:D:82:LYS:C	2.42	0.62
1:E:262:GLN:NE2	2:F:75:LYS:H	1.97	0.62
1:G:346:GLU:HG3	1:G:347:ASN:H	1.65	0.62
1:G:212:ILE:CG2	1:G:243:ILE:HG13	2.29	0.62
1:A:230:GLN:C	1:A:231:ASP:CG	2.67	0.62
1:A:223:SER:HB3	1:A:240:PHE:CD1	2.35	0.61
1:E:394:ASN:O	1:E:397:THR:O	2.18	0.61
1:C:394:ASN:O	1:C:397:THR:O	2.17	0.61
1:A:397:THR:O	1:A:399:GLU:N	2.33	0.61
1:G:222:PHE:HB3	1:G:241:VAL:HG13	1.82	0.61
2:D:81:PHE:O	2:D:82:LYS:O	2.18	0.61
1:C:355:HIS:CG	1:C:356:ARG:H	2.18	0.61
1:C:374:PRO:HD2	1:C:378:MET:CE	2.30	0.61
1:G:290:LYS:HE3	1:G:409:GLU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:GLN:NE2	1:G:398:GLN:CA	2.60	0.61
1:G:314:GLU:HG3	1:G:351:LEU:HD23	1.82	0.61
1:A:238:HIS:O	1:A:239:LEU:HD23	2.00	0.61
1:E:242:HIS:C	1:E:243:ILE:O	2.40	0.60
1:E:261:ARG:HH11	1:E:261:ARG:HB2	1.66	0.60
2:D:55:ASN:C	3:D:130:HOH:O	2.44	0.60
1:A:238:HIS:C	1:A:239:LEU:CG	2.75	0.60
1:C:329:SER:O	1:C:330:PHE:HB2	2.00	0.60
1:E:232:PRO:CA	1:E:233:ASP:HB2	2.32	0.60
1:E:246:SER:CA	1:E:248:PRO:HD3	2.31	0.60
1:G:211:SER:OG	1:G:243:ILE:HG21	2.01	0.60
2:D:71:MET:HE2	2:D:74:ARG:CD	2.32	0.60
2:D:78:ASP:OD2	2:D:78:ASP:N	2.32	0.59
1:A:236:ASN:C	1:A:237:LYS:NZ	2.60	0.59
1:C:260:ILE:HD12	1:C:424:LEU:HD13	1.84	0.59
1:A:345:TYR:CZ	1:A:347:ASN:O	2.56	0.59
1:E:261:ARG:HH11	1:E:261:ARG:CB	2.15	0.59
2:H:71:MET:C	2:H:72:ARG:O	2.39	0.59
1:C:261:ARG:CG	1:C:261:ARG:NH1	2.49	0.58
1:E:275:LYS:HE3	1:E:279:GLU:OE1	2.03	0.58
1:C:259:ASP:OD2	1:C:261:ARG:NH1	2.34	0.58
1:A:229:GLN:C	1:A:230:GLN:CG	2.72	0.58
1:A:270:LYS:HB3	1:A:271:LYS:HD2	1.85	0.58
1:A:356:ARG:O	1:A:357:SER:C	2.47	0.58
2:H:73:LEU:O	2:H:74:ARG:HG3	2.03	0.57
1:A:239:LEU:HD13	1:A:291:PHE:CD1	2.39	0.57
2:D:78:ASP:C	2:D:80:PHE:H	2.10	0.57
2:D:78:ASP:C	2:D:80:PHE:N	2.60	0.57
1:C:355:HIS:C	3:C:174:HOH:O	2.47	0.57
1:A:281:GLY:HA3	3:A:48:HOH:O	2.04	0.57
1:E:325:THR:HG21	3:E:90:HOH:O	2.04	0.57
1:G:288:LEU:HD11	1:G:407:VAL:HG23	1.85	0.57
1:G:356:ARG:NH1	3:G:185:HOH:O	2.36	0.57
1:G:227:GLU:CD	1:G:307:TYR:N	2.63	0.57
2:H:80:PHE:O	2:H:80:PHE:HD1	1.85	0.57
1:A:231:ASP:OD2	1:A:231:ASP:N	2.37	0.57
1:C:214:SER:OG	1:C:216:LYS:N	2.36	0.57
1:A:241:VAL:HG23	1:A:242:HIS:N	2.19	0.56
1:C:212:ILE:HG23	1:C:243:ILE:CD1	2.34	0.56
2:D:71:MET:HE1	2:D:74:ARG:CZ	2.33	0.56
1:E:318:ASN:OD1	1:E:318:ASN:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:GLN:HE21	1:G:353:ARG:HB3	1.69	0.56
2:B:60:PRO:HD2	2:B:61:LYS:H	1.69	0.56
1:E:262:GLN:HE21	2:F:74:ARG:HB3	1.70	0.56
1:E:347:ASN:OD1	1:E:347:ASN:O	2.24	0.56
1:E:375:GLU:HB2	1:E:378:MET:HE3	1.86	0.56
2:B:82:LYS:O	2:B:83:PRO:C	2.49	0.56
2:D:72:ARG:HA	2:D:81:PHE:CE2	2.41	0.55
1:A:223:SER:HB3	1:A:240:PHE:HD1	1.71	0.55
1:A:276:GLU:O	1:A:279:GLU:HG3	2.06	0.55
1:C:240:PHE:HD1	1:C:241:VAL:N	2.04	0.55
1:A:363:MET:O	1:A:367:ILE:HG13	2.07	0.55
1:C:218:TRP:HE1	1:C:243:ILE:CG2	2.16	0.55
1:A:231:ASP:HB2	1:A:232:PRO:CD	2.35	0.55
1:A:280:ARG:HG2	1:A:281:GLY:N	2.21	0.55
1:E:385:ASN:HB2	2:F:53:LEU:HD21	1.89	0.55
2:F:76:LEU:HB3	2:F:77:PRO:HD3	1.88	0.55
1:E:246:SER:HG	1:E:248:PRO:HG3	1.72	0.55
1:C:344:ARG:HG3	1:C:345:TYR:N	2.22	0.55
2:H:78:ASP:C	2:H:80:PHE:H	2.15	0.55
1:A:394:ASN:HB3	1:A:397:THR:O	2.08	0.54
1:E:275:LYS:HE3	1:E:279:GLU:CD	2.32	0.54
1:A:212:ILE:HD13	1:A:212:ILE:O	2.06	0.54
1:E:240:PHE:HZ	1:E:243:ILE:HG22	1.72	0.54
1:E:295:LEU:H	1:E:295:LEU:HD23	1.71	0.54
1:E:345:TYR:CZ	1:E:346:GLU:O	2.60	0.54
1:G:255:LEU:HD12	1:G:421:ILE:HG22	1.88	0.54
1:A:231:ASP:CB	1:A:232:PRO:CD	2.86	0.54
1:A:270:LYS:O	1:A:271:LYS:CD	2.55	0.54
1:E:280:ARG:O	1:E:280:ARG:HG2	2.08	0.54
1:G:232:PRO:HD3	3:G:73:HOH:O	2.08	0.54
1:C:262:GLN:NE2	2:D:74:ARG:HB2	2.23	0.54
1:E:292:TRP:HB3	1:E:411:SER:HB3	1.89	0.54
1:G:371:LYS:HB2	1:G:371:LYS:NZ	2.23	0.53
1:A:343:ALA:HB1	1:A:350:TYR:HB3	1.90	0.53
1:A:397:THR:O	1:A:397:THR:OG1	2.27	0.53
1:C:244:SER:OG	1:C:245:GLN:N	2.42	0.53
1:C:288:LEU:C	1:C:288:LEU:HD23	2.34	0.53
2:D:71:MET:HE2	2:D:74:ARG:NE	2.22	0.53
1:E:247:SER:N	1:E:248:PRO:CD	2.65	0.53
1:C:265:ASP:OD1	3:C:431:HOH:O	2.19	0.53
1:E:377:TYR:CD2	1:E:377:TYR:C	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:260:ILE:HG13	1:G:425:VAL:O	2.09	0.53
2:B:48:THR:C	2:B:50:LEU:N	2.65	0.53
1:E:245:GLN:CD	1:E:245:GLN:O	2.52	0.53
1:E:345:TYR:CE1	1:E:346:GLU:O	2.62	0.53
1:A:229:GLN:O	1:A:230:GLN:HB3	2.08	0.52
1:G:209:MET:HG2	1:G:254:TYR:CD2	2.44	0.52
1:E:263:ILE:HD11	2:F:71:MET:HE3	1.91	0.52
1:C:214:SER:HG	1:C:217:LEU:N	2.07	0.52
2:D:71:MET:HE1	2:D:74:ARG:NE	2.24	0.52
2:F:73:LEU:HD22	2:F:73:LEU:C	2.33	0.52
1:A:353:ARG:HB3	1:G:344:ARG:HH22	1.73	0.52
1:C:226:LEU:HD13	1:C:307:TYR:CZ	2.44	0.52
1:E:217:LEU:HD23	1:E:314:GLU:O	2.10	0.52
1:A:372:HIS:O	1:A:373:LEU:HD23	2.10	0.52
1:E:260:ILE:HG12	1:E:264:TYR:CE1	2.45	0.52
1:E:329:SER:O	1:E:385:ASN:O	2.28	0.52
1:A:372:HIS:O	1:A:372:HIS:CD2	2.63	0.51
1:C:259:ASP:OD1	1:C:259:ASP:C	2.53	0.51
2:B:54:PHE:O	2:B:58:MET:HB2	2.11	0.51
1:C:219:MET:O	1:C:243:ILE:HD12	2.11	0.51
1:G:321:ILE:HG22	1:G:341:GLU:HB2	1.92	0.51
1:A:343:ALA:HB2	1:A:352:TYR:CE1	2.44	0.51
1:C:209:MET:HG2	1:C:423:ARG:HD3	1.91	0.51
1:C:262:GLN:HE22	2:D:74:ARG:HB2	1.75	0.51
1:A:219:MET:HE3	1:A:313:TYR:CE1	2.45	0.51
1:G:345:TYR:CG	1:G:346:GLU:O	2.63	0.51
1:A:270:LYS:HB3	1:A:271:LYS:CD	2.41	0.51
1:A:374:PRO:HG2	1:A:378:MET:SD	2.50	0.51
1:A:270:LYS:CB	1:A:271:LYS:HD2	2.41	0.51
1:A:412:ALA:O	1:A:413:SER:C	2.53	0.51
1:G:268:PRO:HD3	3:G:44:HOH:O	2.10	0.51
1:A:239:LEU:CD1	1:A:408:PHE:HE2	2.24	0.51
2:B:47:GLU:HB3	3:B:171:HOH:O	2.11	0.51
2:B:60:PRO:CD	2:B:61:LYS:H	2.24	0.51
1:C:271:LYS:HG3	1:C:272:GLY:H	1.75	0.50
1:E:260:ILE:HD11	1:E:274:LEU:CD2	2.39	0.50
1:E:393:THR:HG22	1:E:400:THR:HA	1.93	0.50
1:A:212:ILE:HG22	1:A:243:ILE:CD1	2.37	0.50
1:C:357:SER:C	3:C:428:HOH:O	2.55	0.50
1:G:357:SER:CB	1:G:358:PRO:CA	2.89	0.50
1:G:410:VAL:HG12	1:G:411:SER:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:MET:HE3	1:C:313:TYR:CE1	2.47	0.50
1:G:239:LEU:HD22	1:G:291:PHE:CG	2.47	0.50
1:C:252:ASP:N	1:C:253:PRO:CD	2.74	0.50
1:C:219:MET:HE3	1:C:313:TYR:HE1	1.77	0.50
1:E:240:PHE:CZ	1:E:243:ILE:CG2	2.82	0.50
1:A:218:TRP:CD1	1:A:218:TRP:C	2.89	0.49
1:G:278:PHE:HE1	1:G:426:LYS:HB2	1.77	0.49
1:G:239:LEU:HD22	1:G:291:PHE:CD1	2.48	0.49
1:A:370:LEU:HD11	1:A:383:LEU:HD21	1.95	0.49
1:G:295:LEU:O	1:G:371:LYS:HE3	2.13	0.49
2:D:78:ASP:O	2:D:79:SER:C	2.56	0.49
1:E:394:ASN:C	1:E:394:ASN:OD1	2.54	0.49
1:G:381:SER:O	1:G:384:GLU:HB2	2.13	0.49
1:E:410:VAL:HG12	1:E:411:SER:N	2.28	0.49
1:G:315:SER:OG	1:G:319:MET:HE2	2.13	0.49
1:G:378:MET:O	1:G:382:VAL:HG23	2.13	0.49
2:D:72:ARG:HB2	2:D:81:PHE:CZ	2.46	0.49
1:A:271:LYS:O	1:A:276:GLU:OE2	2.30	0.49
1:G:355:HIS:C	1:G:356:ARG:HG3	2.36	0.48
1:E:259:ASP:OD1	1:E:261:ARG:NH1	2.42	0.48
1:E:297:THR:O	1:E:297:THR:CG2	2.60	0.48
1:A:418:GLN:HG2	2:B:84:PRO:HG2	1.95	0.48
1:C:252:ASP:N	1:C:253:PRO:HD3	2.28	0.48
1:E:326:LYS:HG2	1:E:336:GLU:HB2	1.96	0.48
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.54	0.48
1:E:301:ASP:O	1:E:302:GLU:HB2	2.13	0.48
1:E:379:MET:HE3	1:E:410:VAL:HG21	1.94	0.48
1:G:398:GLN:HE21	1:G:398:GLN:CA	2.23	0.48
1:A:326:LYS:HE2	1:A:333:GLN:NE2	2.29	0.48
1:C:217:LEU:HD12	1:C:401:LEU:HB3	1.96	0.47
1:E:425:VAL:O	1:E:426:LYS:HB2	2.12	0.47
2:H:78:ASP:O	2:H:80:PHE:N	2.47	0.47
1:C:240:PHE:CD1	1:C:240:PHE:C	2.91	0.47
2:D:49:ASP:HA	3:D:142:HOH:O	2.14	0.47
1:G:307:TYR:O	1:G:358:PRO:HG3	2.12	0.47
1:A:394:ASN:O	1:A:397:THR:O	2.32	0.47
1:A:290:LYS:O	1:A:419:HIS:HA	2.15	0.47
1:A:212:ILE:O	1:A:212:ILE:HG23	2.15	0.47
1:G:209:MET:HG2	1:G:254:TYR:CE2	2.50	0.47
1:G:325:THR:HG22	3:G:62:HOH:O	2.15	0.47
2:H:78:ASP:C	2:H:80:PHE:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLN:NE2	2:B:75:LYS:HG3	2.30	0.47
1:A:262:GLN:O	2:B:74:ARG:NH1	2.42	0.47
1:C:252:ASP:HB2	3:C:22:HOH:O	2.13	0.47
2:D:49:ASP:HB2	3:D:24:HOH:O	2.14	0.47
1:C:263:ILE:HD12	1:C:263:ILE:HA	1.75	0.47
1:C:375:GLU:HB2	1:C:378:MET:HG3	1.97	0.47
1:E:295:LEU:HD23	1:E:295:LEU:N	2.28	0.47
1:E:301:ASP:O	1:E:302:GLU:CB	2.63	0.47
1:G:281:GLY:HA3	1:G:400:THR:CG2	2.45	0.47
1:A:260:ILE:HG13	1:A:264:TYR:CE1	2.50	0.47
1:A:271:LYS:HD2	1:A:271:LYS:N	2.29	0.47
1:A:373:LEU:HD22	1:A:374:PRO:HD2	1.97	0.47
1:E:217:LEU:CD2	1:E:313:TYR:HB3	2.45	0.47
1:C:259:ASP:O	1:C:260:ILE:C	2.57	0.46
1:C:355:HIS:HB3	3:C:174:HOH:O	2.15	0.46
2:D:72:ARG:CB	2:D:81:PHE:CZ	2.98	0.46
1:A:344:ARG:NH2	1:G:353:ARG:HG3	2.30	0.46
1:A:356:ARG:O	1:A:357:SER:O	2.32	0.46
1:C:267:PHE:CZ	1:C:405:ALA:HB1	2.50	0.46
1:E:353:ARG:HD2	1:E:353:ARG:O	2.14	0.46
1:E:385:ASN:HD21	2:F:68:THR:HG21	1.79	0.46
1:C:363:MET:O	1:C:367:ILE:HG12	2.15	0.46
1:A:294:ASP:HB2	1:A:417:ALA:HB2	1.98	0.46
2:F:49:ASP:HA	3:F:179:HOH:O	2.15	0.46
1:A:211:SER:OG	1:A:243:ILE:HG21	2.15	0.46
1:E:222:PHE:C	1:E:222:PHE:CD2	2.93	0.46
1:A:232:PRO:HB3	1:G:236:ASN:HA	1.97	0.46
1:C:326:LYS:HD3	1:C:333:GLN:NE2	2.30	0.46
1:E:226:LEU:HG	1:E:299:ILE:HD11	1.97	0.46
1:C:232:PRO:HG2	1:E:234:THR:HG23	1.98	0.46
1:E:295:LEU:HD21	1:E:410:VAL:HG22	1.98	0.46
1:E:315:SER:OG	1:E:319:MET:HE2	2.16	0.46
2:B:56:ALA:HB2	2:B:65:VAL:HG21	1.98	0.46
1:A:328:CYS:HB3	1:A:332:LYS:O	2.15	0.45
1:E:218:TRP:HZ2	1:E:246:SER:OG	2.00	0.45
2:B:59:ASN:N	2:B:60:PRO:CA	2.77	0.45
2:D:78:ASP:O	2:D:80:PHE:N	2.49	0.45
1:E:353:ARG:HD2	1:E:353:ARG:C	2.41	0.45
1:G:251:SER:N	3:G:17:HOH:O	2.49	0.45
1:A:407:VAL:HG11	2:B:80:PHE:HZ	1.82	0.45
1:C:228:ARG:HD2	1:C:228:ARG:HA	1.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:HIS:O	1:C:372:HIS:HD2	1.99	0.45
1:E:236:ASN:ND2	3:E:148:HOH:O	2.38	0.45
1:E:263:ILE:HD11	2:F:71:MET:CE	2.47	0.45
1:G:268:PRO:HD2	3:G:205:HOH:O	2.16	0.45
1:E:212:ILE:HG23	1:E:212:ILE:O	2.16	0.45
1:E:245:GLN:O	1:E:245:GLN:OE1	2.34	0.45
1:C:355:HIS:CG	1:C:356:ARG:N	2.80	0.45
1:E:252:ASP:HB3	1:E:253:PRO:HD2	1.97	0.45
1:E:418:GLN:HA	3:E:167:HOH:O	2.17	0.45
1:G:252:ASP:HB3	1:G:253:PRO:HG3	1.97	0.45
1:A:320:ILE:O	1:A:395:ARG:HB2	2.17	0.45
2:D:72:ARG:CA	2:D:81:PHE:CZ	2.99	0.45
2:D:77:PRO:O	2:D:80:PHE:HB2	2.16	0.45
2:F:72:ARG:H	2:F:72:ARG:HG2	1.35	0.45
1:E:370:LEU:HD12	2:F:54:PHE:CZ	2.52	0.45
1:G:232:PRO:CD	3:G:73:HOH:O	2.63	0.44
1:G:381:SER:HA	1:G:384:GLU:HG3	2.00	0.44
1:E:259:ASP:OD2	1:E:259:ASP:C	2.59	0.44
1:A:315:SER:HB3	1:A:352:TYR:HE2	1.82	0.44
1:E:241:VAL:CG1	1:E:242:HIS:N	2.81	0.44
1:E:345:TYR:CD1	1:E:345:TYR:C	2.95	0.44
1:G:393:THR:HG22	1:G:400:THR:HA	2.00	0.44
1:A:355:HIS:C	1:A:357:SER:N	2.74	0.44
2:B:76:LEU:HB3	2:B:77:PRO:HD2	1.97	0.44
1:E:361:GLU:HA	1:E:364:ILE:HD12	2.00	0.44
2:F:59:ASN:HB3	2:F:62:THR:HG23	1.99	0.44
1:G:346:GLU:CD	1:G:351:LEU:HD11	2.42	0.44
1:G:357:SER:H	1:G:358:PRO:HD3	1.79	0.44
1:C:240:PHE:HD1	1:C:240:PHE:C	2.26	0.44
1:G:355:HIS:C	1:G:356:ARG:CG	2.91	0.44
1:G:280:ARG:C	1:G:280:ARG:CD	2.69	0.44
2:B:71:MET:C	2:B:73:LEU:H	2.26	0.44
2:B:82:LYS:C	2:B:83:PRO:O	2.58	0.44
1:C:294:ASP:OD1	1:C:294:ASP:C	2.58	0.43
2:B:47:GLU:C	2:B:49:ASP:H	2.26	0.43
2:D:54:PHE:C	2:D:56:ALA:H	2.25	0.43
1:C:426:LYS:NZ	1:C:426:LYS:CB	2.72	0.43
1:G:211:SER:OG	1:G:212:ILE:N	2.51	0.43
1:G:226:LEU:O	1:G:235:TYR:CB	2.53	0.43
1:E:278:PHE:HA	1:E:286:PHE:CZ	2.53	0.43
2:H:72:ARG:O	2:H:73:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:HIS:CD2	1:C:356:ARG:H	2.36	0.43
1:G:243:ILE:CG2	1:G:244:SER:N	2.79	0.43
1:G:410:VAL:HG12	1:G:411:SER:H	1.84	0.43
1:A:243:ILE:HG22	1:A:243:ILE:O	2.18	0.43
1:C:308:GLY:HA2	3:C:428:HOH:O	2.18	0.43
2:B:65:VAL:HB	2:B:66:PRO:HD2	2.00	0.43
1:E:228:ARG:HH12	1:E:304:SER:HB3	1.84	0.43
1:E:267:PHE:CZ	1:E:405:ALA:HB1	2.54	0.43
1:G:345:TYR:CE1	1:G:346:GLU:O	2.72	0.43
1:A:383:LEU:O	1:A:384:GLU:C	2.62	0.42
1:E:231:ASP:N	3:E:186:HOH:O	2.48	0.42
2:F:50:LEU:C	2:F:52:ALA:N	2.77	0.42
1:G:267:PHE:HA	1:G:268:PRO:HA	1.76	0.42
1:A:231:ASP:CG	1:A:232:PRO:HD3	2.44	0.42
1:C:260:ILE:HG23	1:C:261:ARG:N	2.35	0.42
1:E:261:ARG:CG	1:E:261:ARG:NH1	2.62	0.42
1:A:269:GLU:O	1:A:273:GLY:HA3	2.19	0.42
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.91	0.42
2:B:85:GLU:HG3	3:B:35:HOH:O	2.19	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD2	1.83	0.42
2:B:78:ASP:C	2:B:80:PHE:H	2.28	0.42
2:D:72:ARG:O	2:D:72:ARG:HG3	2.13	0.42
1:E:346:GLU:HG2	1:E:347:ASN:OD1	2.19	0.42
1:G:243:ILE:HG22	1:G:244:SER:H	1.84	0.42
2:D:82:LYS:HE3	2:D:82:LYS:HB2	1.67	0.42
1:A:212:ILE:C	1:A:212:ILE:CD1	2.91	0.42
1:A:328:CYS:HB3	1:A:332:LYS:C	2.44	0.42
1:A:380:ASN:ND2	1:A:409:GLU:HG2	2.35	0.42
1:C:300:ASP:OD1	1:C:368:HIS:HE1	2.03	0.42
1:A:278:PHE:HA	1:A:286:PHE:CZ	2.55	0.41
1:G:209:MET:CG	1:G:254:TYR:HD2	2.33	0.41
1:E:217:LEU:HD22	1:E:313:TYR:HB3	2.01	0.41
1:E:343:ALA:HB2	1:E:352:TYR:CE1	2.55	0.41
2:B:60:PRO:C	3:B:176:HOH:O	2.63	0.41
1:G:237:LYS:NZ	1:G:237:LYS:CB	2.58	0.41
1:C:426:LYS:HB2	1:C:426:LYS:HZ3	1.82	0.41
1:E:231:ASP:CB	3:E:26:HOH:O	2.36	0.41
1:E:267:PHE:HB3	1:E:268:PRO:HD2	2.03	0.41
1:A:236:ASN:C	1:A:237:LYS:HZ1	2.27	0.41
1:A:239:LEU:HD11	1:A:408:PHE:HE2	1.84	0.41
1:E:275:LYS:HE3	1:E:279:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:TYR:N	1:E:352:TYR:CD2	2.87	0.41
1:A:239:LEU:HD23	1:A:239:LEU:HA	1.35	0.41
2:B:53:LEU:HD23	2:B:53:LEU:HA	1.82	0.41
1:C:260:ILE:HG12	1:C:264:TYR:CE1	2.55	0.41
1:C:361:GLU:O	1:C:362:TYR:C	2.61	0.41
1:C:388:ILE:HD12	1:C:408:PHE:CZ	2.56	0.41
1:E:236:ASN:CG	1:E:297:THR:HB	2.44	0.41
1:A:212:ILE:O	1:A:212:ILE:CD1	2.69	0.41
1:E:212:ILE:HD11	1:E:404:ILE:HG12	2.03	0.41
2:F:55:ASN:O	2:F:56:ALA:C	2.63	0.41
1:G:265:ASP:OD1	2:H:74:ARG:NH2	2.53	0.41
1:G:314:GLU:HG3	1:G:351:LEU:CD2	2.48	0.41
2:B:78:ASP:C	2:B:80:PHE:N	2.77	0.41
1:C:356:ARG:NE	3:C:158:HOH:O	2.54	0.41
1:E:263:ILE:HD12	1:E:263:ILE:HA	1.85	0.41
1:G:214:SER:HB3	1:G:401:LEU:O	2.21	0.41
2:H:72:ARG:O	2:H:73:LEU:CB	2.69	0.41
1:A:230:GLN:O	1:A:232:PRO:N	2.54	0.41
1:A:380:ASN:CG	1:A:409:GLU:HG2	2.46	0.40
1:C:230:GLN:C	1:C:231:ASP:O	2.60	0.40
1:E:236:ASN:ND2	1:E:297:THR:HB	2.36	0.40
1:E:426:LYS:HZ3	1:E:426:LYS:HG3	1.64	0.40
1:A:327:VAL:HB	1:A:335:VAL:HG13	2.03	0.40
2:B:80:PHE:O	2:B:80:PHE:CD2	2.75	0.40
1:G:226:LEU:HD23	1:G:297:THR:HG21	2.04	0.40
2:H:75:LYS:C	2:H:76:LEU:CD2	2.58	0.40
1:C:226:LEU:HD13	1:C:307:TYR:CE2	2.57	0.40
1:C:376:LYS:CA	1:C:379:MET:HE3	2.41	0.40
2:D:69:VAL:HA	2:D:70:PRO:HD2	1.85	0.40
1:E:226:LEU:HD13	1:E:307:TYR:CZ	2.56	0.40
1:G:402:LEU:HD22	1:G:402:LEU:HA	1.95	0.40
1:A:219:MET:HE3	1:A:313:TYR:HE1	1.87	0.40
1:E:232:PRO:CB	1:E:233:ASP:CB	2.88	0.40
1:E:343:ALA:HB1	1:E:350:TYR:HB3	2.04	0.40
1:E:238:HIS:O	1:E:239:LEU:HD13	2.21	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	196/220 (89%)	173 (88%)	16 (8%)	7 (4%)	2	16
1	C	209/220 (95%)	189 (90%)	18 (9%)	2 (1%)	12	45
1	E	212/220 (96%)	189 (89%)	16 (8%)	7 (3%)	3	17
1	G	178/220 (81%)	164 (92%)	10 (6%)	4 (2%)	5	26
2	B	37/39 (95%)	32 (86%)	4 (11%)	1 (3%)	4	22
2	D	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
2	F	34/39 (87%)	25 (74%)	8 (24%)	1 (3%)	3	20
2	H	17/39 (44%)	10 (59%)	5 (29%)	2 (12%)	0	1
All	All	916/1036 (88%)	812 (89%)	80 (9%)	24 (3%)	4	23

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	231	ASP
1	A	271	LYS
1	C	358	PRO
1	E	244	SER
1	G	253	PRO
1	G	357	SER
1	A	356	ARG
1	A	357	SER
2	F	60	PRO
2	H	79	SER
1	A	398	GLN
1	E	242	HIS
1	C	356	ARG
1	E	233	ASP
1	E	231	ASP
1	G	252	ASP

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Mol	Chain	Res	Type
2	H	70	PRO
1	E	232	PRO
1	A	232	PRO
1	E	243	ILE
2	B	60	PRO
1	G	212	ILE
1	E	212	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	188/203 (93%)	163 (87%)	25 (13%)	4	18
1	C	196/203 (97%)	167 (85%)	29 (15%)	3	15
1	E	200/203 (98%)	168 (84%)	32 (16%)	2	12
1	G	178/203 (88%)	151 (85%)	27 (15%)	3	14
2	B	36/36 (100%)	28 (78%)	8 (22%)	1	5
2	D	32/36 (89%)	25 (78%)	7 (22%)	1	5
2	F	33/36 (92%)	28 (85%)	5 (15%)	3	14
2	H	19/36 (53%)	14 (74%)	5 (26%)	0	3
All	All	882/956 (92%)	744 (84%)	138 (16%)	2	13

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ILE
1	A	217	LEU
1	A	228	ARG
1	A	231	ASP
1	A	234	THR
1	A	235	TYR
1	A	237	LYS
1	A	241	VAL

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Mol	Chain	Res	Type
1	A	242	HIS
1	A	274	LEU
1	A	298	ASN
1	A	309	VAL
1	A	314	GLU
1	A	325	THR
1	A	328	CYS
1	A	335	VAL
1	A	339	GLU
1	A	354	ILE
1	A	360	CYS
1	A	381	SER
1	A	389	LEU
1	A	395	ARG
1	A	398	GLN
1	A	401	LEU
1	A	418	GLN
2	B	49	ASP
2	B	50	LEU
2	B	51	GLU
2	B	61	LYS
2	B	68	THR
2	B	69	VAL
2	B	72	ARG
2	B	78	ASP
1	C	210	ARG
1	C	212	ILE
1	C	217	LEU
1	C	221	GLU
1	C	230	GLN
1	C	234	THR
1	C	235	TYR
1	C	239	LEU
1	C	245	GLN
1	C	254	TYR
1	C	260	ILE
1	C	261	ARG
1	C	263	ILE
1	C	269	GLU
1	C	271	LYS
1	C	283	SER
1	C	324	SER

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Mol	Chain	Res	Type
1	C	325	THR
1	C	333	GLN
1	C	346	GLU
1	C	353	ARG
1	C	356	ARG
1	C	369	LYS
1	C	371	LYS
1	C	384	GLU
1	C	389	LEU
1	C	395	ARG
1	C	398	GLN
1	C	426	LYS
2	D	57	VAL
2	D	69	VAL
2	D	72	ARG
2	D	73	LEU
2	D	74	ARG
2	D	78	ASP
2	D	79	SER
1	E	217	LEU
1	E	226	LEU
1	E	229	GLN
1	E	230	GLN
1	E	244	SER
1	E	245	GLN
1	E	246	SER
1	E	261	ARG
1	E	263	ILE
1	E	271	LYS
1	E	274	LEU
1	E	277	LEU
1	E	295	LEU
1	E	298	ASN
1	E	299	ILE
1	E	312	GLN
1	E	319	MET
1	E	320	ILE
1	E	322	THR
1	E	329	SER
1	E	336	GLU
1	E	339	GLU
1	E	340	THR

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Mol	Chain	Res	Type
1	E	346	GLU
1	E	347	ASN
1	E	354	ILE
1	E	372	HIS
1	E	379	MET
1	E	389	LEU
1	E	398	GLN
1	E	401	LEU
1	E	426	LYS
2	F	57	VAL
2	F	62	THR
2	F	65	VAL
2	F	69	VAL
2	F	73	LEU
1	G	217	LEU
1	G	227	GLU
1	G	230	GLN
1	G	235	TYR
1	G	237	LYS
1	G	239	LEU
1	G	241	VAL
1	G	252	ASP
1	G	260	ILE
1	G	269	GLU
1	G	295	LEU
1	G	297	THR
1	G	312	GLN
1	G	321	ILE
1	G	344	ARG
1	G	358	PRO
1	G	360	CYS
1	G	371	LYS
1	G	375	GLU
1	G	384	GLU
1	G	389	LEU
1	G	395	ARG
1	G	398	GLN
1	G	401	LEU
1	G	402	LEU
1	G	404	ILE
1	G	420	HIS
2	H	69	VAL

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Mol	Chain	Res	Type
2	H	73	LEU
2	H	74	ARG
2	H	76	LEU
2	H	79	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	GLN
1	A	333	GLN
1	A	347	ASN
1	A	349	HIS
1	A	365	ASN
1	A	372	HIS
1	A	380	ASN
1	A	385	ASN
1	A	390	GLN
1	A	398	GLN
2	B	55	ASN
1	C	229	GLN
1	C	236	ASN
1	C	238	HIS
1	C	242	HIS
1	C	262	GLN
1	C	333	GLN
1	C	347	ASN
1	C	368	HIS
1	C	372	HIS
1	C	385	ASN
2	D	55	ASN
1	E	236	ASN
1	E	262	GLN
1	E	298	ASN
1	E	365	ASN
1	E	385	ASN
1	E	398	GLN
1	G	229	GLN
1	G	284	ASN
1	G	312	GLN
1	G	349	HIS
1	G	368	HIS
1	G	398	GLN

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Mol	Chain	Res	Type
1	G	419	HIS
1	G	420	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	204/220 (92%)	-0.25	3 (1%) 72 49	15, 25, 35, 43	0
1	C	213/220 (96%)	-0.07	8 (3%) 44 24	18, 28, 39, 53	0
1	E	216/220 (98%)	0.04	8 (3%) 45 25	19, 28, 40, 60	0
1	G	190/220 (86%)	0.33	13 (6%) 23 12	14, 28, 39, 43	0
2	B	39/39 (100%)	0.37	3 (7%) 19 10	21, 25, 36, 36	0
2	D	35/39 (89%)	0.09	2 (5%) 29 15	25, 28, 37, 39	0
2	F	36/39 (92%)	1.38	10 (27%) 1 1	26, 32, 39, 39	0
2	H	19/39 (48%)	0.99	3 (15%) 5 3	21, 27, 34, 34	0
All	All	952/1036 (91%)	0.10	50 (5%) 32 16	14, 28, 39, 60	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	65	VAL	5.5
1	G	231	ASP	5.1
1	E	244	SER	5.1
2	F	61	LYS	5.0
1	G	359	LEU	3.9
2	D	48	THR	3.8
1	G	208	SER	3.8
1	C	232	PRO	3.6
1	G	229	GLN	3.5
1	E	246	SER	3.4
2	B	60	PRO	3.4
1	C	231	ASP	3.3
2	F	82	LYS	3.1
1	E	230	GLN	3.1
1	G	232	PRO	3.1
1	A	208	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	272	GLY	3.1
2	B	85	GLU	3.0
1	G	251	SER	3.0
2	F	75	LYS	3.0
1	C	243	ILE	2.9
2	F	48	THR	2.8
1	C	230	GLN	2.8
1	E	245	GLN	2.8
1	E	243	ILE	2.8
1	A	235	TYR	2.7
1	E	298	ASN	2.7
2	H	83	PRO	2.7
2	F	79	SER	2.6
2	F	83	PRO	2.6
1	C	357	SER	2.4
2	B	61	LYS	2.3
2	F	80	PHE	2.3
1	C	245	GLN	2.3
1	E	302	GLU	2.3
2	D	82	LYS	2.3
1	G	358	PRO	2.3
1	G	348	GLY	2.2
1	A	242	HIS	2.2
2	F	58	MET	2.2
1	G	268	PRO	2.2
2	F	81	PHE	2.2
1	G	235	TYR	2.1
1	G	233	ASP	2.1
1	G	272	GLY	2.1
1	G	218	TRP	2.1
2	H	68	THR	2.1
1	C	208	SER	2.1
1	E	235	TYR	2.0
2	F	76	LEU	2.0

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

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

6.3 Carbohydrates [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.