



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 11:59 PM UTC

PDB ID : 1FT8 / pdb_00001ft8
Title : CRYSTAL STRUCTURE OF THE RNA-BINDING DOMAIN OF THE MRNA EXPORT FACTOR TAP
Authors : Liker, E.; Fernandez, E.; Izaurralde, E.; Conti, E.
Deposited on : 2000-09-12
Resolution : 3.15 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

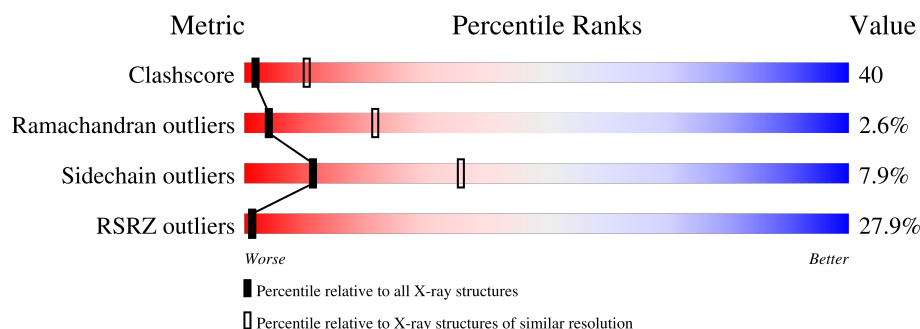
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	271	21% 40% 38% 9% • 11%
1	B	271	14% 31% 24% 6% 39%
1	C	271	29% 46% 36% 6% • 10%
1	D	271	17% 27% 26% 6% • 40%
1	E	271	8% 5% 8% • • 84%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6913 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 TIP ASSOCIATING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1961	1245	343	366	7			
1	B	165	Total	C	N	O	S	0	0	0
			1323	831	232	255	5			
1	C	244	Total	C	N	O	S	0	0	0
			1973	1253	346	367	7			
1	D	162	Total	C	N	O	S	0	0	0
			1302	818	229	250	5			
1	E	44	Total	C	N	O	S	0	0	0
			354	236	54	62	2			

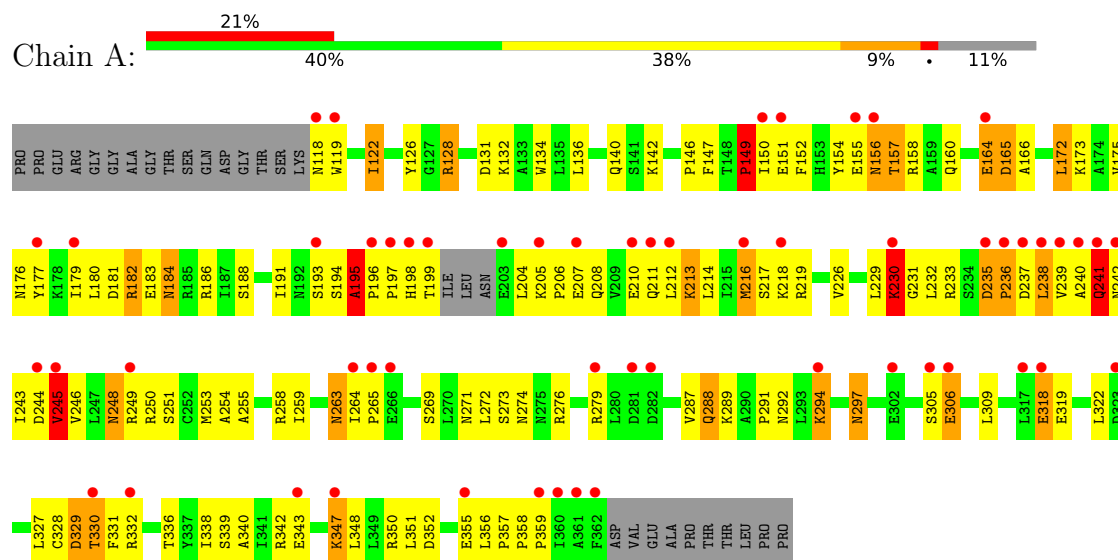
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	TRP	CYS	engineered mutation	UNP Q9UBU9
A	226	VAL	ALA	engineered mutation	UNP Q9UBU9
B	119	TRP	CYS	engineered mutation	UNP Q9UBU9
B	226	VAL	ALA	engineered mutation	UNP Q9UBU9
C	119	TRP	CYS	engineered mutation	UNP Q9UBU9
C	226	VAL	ALA	engineered mutation	UNP Q9UBU9
D	119	TRP	CYS	engineered mutation	UNP Q9UBU9
D	226	VAL	ALA	engineered mutation	UNP Q9UBU9
E	119	TRP	CYS	engineered mutation	UNP Q9UBU9
E	226	VAL	ALA	engineered mutation	UNP Q9UBU9

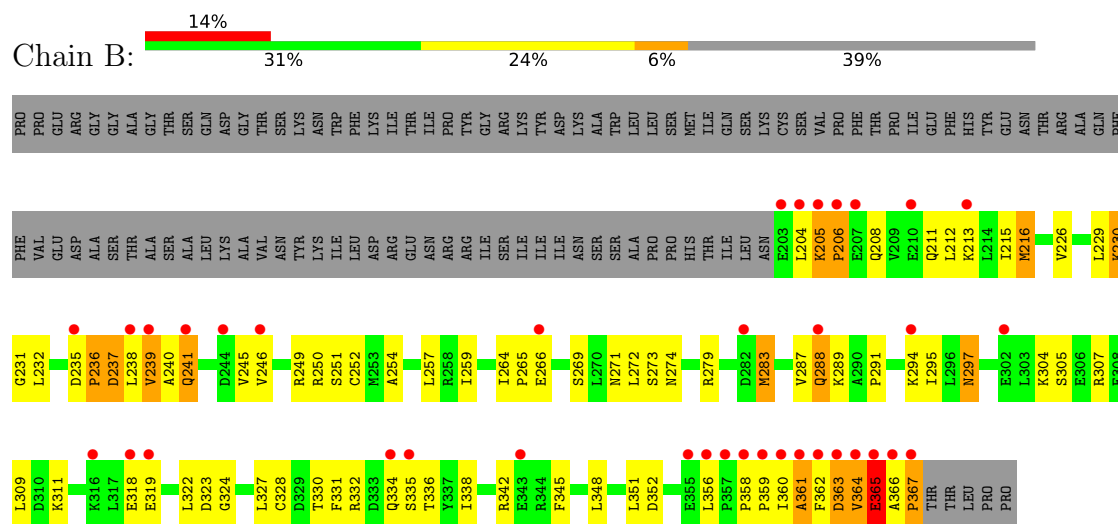
3 Residue-property plots

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: TIP ASSOCIATING PROTEIN



• Molecule 1: TIP ASSOCIATING PROTEIN



• Molecule 1: TIP ASSOCIATING PROTEIN



PRO
LYS
LEU
LEU
ARG
LEU
ASP
GLY
HIS
GLU
LEU
PRO
PRO
PRO
ILE
ALA
PHE
ASP
VAL
GLU
ALA
PRO
THR
THR
LEU
PRO
PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.92Å 139.92Å 206.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15 30.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.15) 99.4 (30.00-3.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.10 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.303 , 0.303 0.296 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.6	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	0.86	EDS
Total number of atoms	6913	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.83	5/1996 (0.3%)	1.27	21/2696 (0.8%)
1	B	0.75	2/1340 (0.1%)	1.17	10/1808 (0.6%)
1	C	0.90	11/2008 (0.5%)	1.17	18/2711 (0.7%)
1	D	0.77	2/1318 (0.2%)	1.22	14/1777 (0.8%)
1	E	0.84	0/363	1.44	7/489 (1.4%)
All	All	0.83	20/7025 (0.3%)	1.22	70/9481 (0.7%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	ASN	CA-C	-10.81	1.38	1.52
1	A	165	ASP	CB-CG	-9.84	1.27	1.52
1	C	242	ASN	CA-CB	9.48	1.69	1.53
1	C	228	ASP	CB-CG	-8.67	1.30	1.52
1	C	165	ASP	CB-CG	-7.71	1.32	1.52
1	A	164	GLU	CB-CG	-6.50	1.32	1.52
1	B	216	MET	SD-CE	-6.44	1.63	1.79
1	C	241	GLN	N-CA	6.43	1.54	1.46
1	A	194	SER	CA-C	-6.38	1.45	1.52
1	B	283	MET	SD-CE	-6.32	1.63	1.79
1	C	242	ASN	N-CA	6.21	1.54	1.46
1	D	216	MET	SD-CE	-6.00	1.64	1.79
1	C	216	MET	SD-CE	-5.97	1.64	1.79
1	A	165	ASP	N-CA	-5.61	1.39	1.46
1	A	216	MET	SD-CE	-5.55	1.65	1.79
1	C	243	ILE	N-CA	5.45	1.52	1.46
1	D	228	ASP	CB-CG	-5.29	1.38	1.52
1	C	244	ASP	CA-C	5.29	1.59	1.52
1	C	164	GLU	CB-CG	-5.05	1.37	1.52
1	C	228	ASP	CA-C	-5.01	1.46	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ALA	CA-C-N	17.35	138.25	120.38
1	A	195	ALA	C-N-CA	17.35	138.25	120.38
1	E	144	SER	CA-C-N	-10.01	103.62	122.13
1	E	144	SER	C-N-CA	-10.01	103.62	122.13
1	A	235	ASP	N-CA-C	9.88	122.52	110.07
1	C	241	GLN	O-C-N	8.95	131.60	122.12
1	A	236	PRO	N-CA-C	-8.43	98.77	111.41
1	C	244	ASP	N-CA-C	8.02	122.35	110.48
1	D	235	ASP	CA-C-N	7.86	129.66	119.84
1	D	235	ASP	C-N-CA	7.86	129.66	119.84
1	A	157	THR	N-CA-C	7.74	121.65	111.75
1	C	228	ASP	CB-CG-OD1	-7.69	100.71	118.40
1	A	165	ASP	CB-CG-OD2	-7.43	101.32	118.40
1	C	236	PRO	N-CA-C	7.41	127.73	112.47
1	C	165	ASP	CB-CG-OD2	-7.20	101.83	118.40
1	A	164	GLU	N-CA-CB	-6.98	100.73	110.65
1	B	205	LYS	CA-C-N	6.97	128.55	119.84
1	B	205	LYS	C-N-CA	6.97	128.55	119.84
1	A	318	GLU	N-CA-C	-6.75	105.33	113.97
1	B	361	ALA	N-CA-C	6.72	120.77	109.76
1	D	253	MET	N-CA-C	-6.68	104.03	111.71
1	A	263	ASN	N-CA-C	6.56	121.56	113.50
1	B	318	GLU	N-CA-C	-6.55	105.02	114.12
1	E	146	PRO	N-CA-C	6.51	125.87	112.47
1	A	241	GLN	CA-C-N	6.41	133.79	121.54
1	A	241	GLN	C-N-CA	6.41	133.79	121.54
1	C	228	ASP	N-CA-CB	6.41	121.11	110.47
1	B	362	PHE	N-CA-C	-6.33	98.58	108.90
1	C	228	ASP	OD1-CG-OD2	6.33	138.09	122.90
1	D	237	ASP	CA-C-N	6.27	133.51	121.54
1	D	237	ASP	C-N-CA	6.27	133.51	121.54
1	D	318	GLU	N-CA-C	-6.21	106.24	113.88
1	D	237	ASP	O-C-N	6.17	130.80	122.59
1	E	145	VAL	CA-C-N	6.17	127.55	119.84
1	E	145	VAL	C-N-CA	6.17	127.55	119.84
1	C	245	VAL	CB-CA-C	-6.17	104.25	111.09
1	C	203	GLU	N-CA-C	-6.08	102.47	110.43
1	A	230	LYS	N-CA-C	5.98	118.38	109.59
1	A	238	LEU	N-CA-C	-5.96	101.53	110.06
1	C	318	GLU	N-CA-C	-5.94	106.36	113.97
1	D	242	ASN	N-CA-C	-5.90	100.92	109.59
1	D	237	ASP	CB-CA-C	5.86	122.09	110.42
1	A	165	ASP	N-CA-CB	-5.84	101.00	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	THR	N-CA-C	5.79	123.14	110.80
1	C	228	ASP	CB-CA-C	-5.66	101.57	110.79
1	A	245	VAL	CA-C-N	-5.63	116.40	122.59
1	A	245	VAL	C-N-CA	-5.63	116.40	122.59
1	E	145	VAL	O-C-N	5.58	127.47	121.10
1	C	149	PRO	CA-C-N	-5.57	115.19	122.37
1	C	149	PRO	C-N-CA	-5.57	115.19	122.37
1	B	345	PHE	CA-C-N	5.54	125.63	119.32
1	B	345	PHE	C-N-CA	5.54	125.63	119.32
1	D	345	PHE	CA-C-N	5.54	125.63	119.32
1	D	345	PHE	C-N-CA	5.54	125.63	119.32
1	A	193	SER	N-CA-C	-5.48	103.15	110.55
1	D	237	ASP	CA-C-O	5.37	128.19	120.51
1	A	253	MET	N-CA-C	-5.34	105.56	111.71
1	B	362	PHE	CA-C-N	5.29	131.65	121.54
1	B	362	PHE	C-N-CA	5.29	131.65	121.54
1	B	239	VAL	N-CA-C	-5.29	105.45	110.42
1	D	208	GLN	N-CA-C	-5.28	105.44	111.14
1	A	184	ASN	N-CA-C	5.27	119.01	112.58
1	C	250	ARG	N-CA-C	5.23	117.39	111.11
1	D	243	ILE	N-CA-C	-5.22	98.48	109.34
1	C	306	GLU	N-CA-C	-5.17	106.80	113.01
1	C	233	ARG	CA-C-N	-5.10	114.17	123.34
1	C	233	ARG	C-N-CA	-5.10	114.17	123.34
1	A	149	PRO	CA-C-N	-5.06	114.67	121.66
1	A	149	PRO	C-N-CA	-5.06	114.67	121.66
1	E	145	VAL	N-CA-C	5.06	119.81	108.88

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	1961	0	2003	175	0
1	B	1323	0	1363	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1973	0	2013	137	0
1	D	1302	0	1345	120	0
1	E	354	0	349	51	1
All	All	6913	0	7073	555	1

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 40.

All (555) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HD2	1:A:273:SER:OG	1.29	1.32
1:B:323:ASP:HB2	1:C:177:TYR:CE2	1.78	1.19
1:C:119:TRP:HZ3	1:C:150:ILE:CD1	1.56	1.19
1:E:144:SER:O	1:E:145:VAL:HG23	1.39	1.19
1:E:145:VAL:HG22	1:E:146:PRO:CD	1.73	1.17
1:C:119:TRP:CZ3	1:C:150:ILE:HD11	1.81	1.15
1:A:238:LEU:HD12	1:A:241:GLN:CB	1.78	1.12
1:A:238:LEU:CD1	1:A:241:GLN:HB3	1.82	1.10
1:E:145:VAL:HG22	1:E:146:PRO:HD3	1.21	1.10
1:E:145:VAL:CG1	1:E:146:PRO:HD2	1.81	1.09
1:E:145:VAL:HG13	1:E:146:PRO:HD2	1.16	1.09
1:A:238:LEU:HD12	1:A:241:GLN:HB2	1.35	1.09
1:A:230:LYS:HA	1:A:230:LYS:HE3	1.34	1.08
1:A:230:LYS:HE2	1:A:273:SER:N	1.65	1.07
1:C:119:TRP:HZ3	1:C:150:ILE:HD11	0.92	1.07
1:A:230:LYS:HA	1:A:230:LYS:CE	1.84	1.05
1:B:204:LEU:HA	1:B:208:GLN:NE2	1.71	1.05
1:B:323:ASP:CB	1:C:177:TYR:HE2	1.68	1.05
1:B:323:ASP:HB2	1:C:177:TYR:HE2	0.96	1.04
1:E:144:SER:O	1:E:145:VAL:CG2	2.07	1.03
1:B:366:ALA:HB3	1:B:367:PRO:HD3	1.32	1.02
1:A:119:TRP:HZ3	1:A:150:ILE:HD11	1.26	1.00
1:A:238:LEU:HD21	1:A:243:ILE:O	1.61	1.00
1:B:238:LEU:HD21	1:B:245:VAL:HG21	1.41	1.00
1:D:235:ASP:HB3	1:D:236:PRO:HD3	1.45	0.99
1:E:145:VAL:HG13	1:E:146:PRO:CD	1.91	0.99
1:C:237:ASP:O	1:C:240:ALA:N	1.96	0.98
1:A:126:TYR:HA	1:A:157:THR:HG22	1.44	0.98
1:B:215:ILE:HG13	1:B:238:LEU:HD13	1.41	0.97
1:A:230:LYS:CD	1:A:273:SER:OG	2.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD11	1:A:241:GLN:HB3	1.44	0.96
1:A:230:LYS:NZ	1:A:271:ASN:O	1.99	0.96
1:C:165:ASP:OD2	1:C:165:ASP:N	1.87	0.95
1:C:237:ASP:O	1:C:239:VAL:N	2.00	0.94
1:E:145:VAL:CG2	1:E:146:PRO:CD	2.47	0.92
1:B:366:ALA:CB	1:B:367:PRO:HD3	1.99	0.92
1:B:366:ALA:HB3	1:B:367:PRO:CD	1.99	0.92
1:B:364:VAL:HG22	1:B:367:PRO:HB2	1.50	0.92
1:C:142:LYS:HD3	1:C:178:LYS:HG2	1.51	0.91
1:A:238:LEU:CD1	1:A:241:GLN:CB	2.44	0.91
1:E:145:VAL:CG2	1:E:146:PRO:HD3	2.00	0.91
1:B:216:MET:HE1	1:B:259:ILE:HD12	1.53	0.89
1:D:235:ASP:O	1:D:237:ASP:N	2.04	0.89
1:D:235:ASP:O	1:D:237:ASP:CG	2.16	0.89
1:C:126:TYR:HA	1:C:157:THR:HG22	1.54	0.89
1:D:216:MET:HE1	1:D:259:ILE:HD12	1.54	0.88
1:C:119:TRP:CZ3	1:C:150:ILE:CD1	2.47	0.88
1:C:164:GLU:OE2	1:C:164:GLU:O	1.92	0.88
1:A:230:LYS:HE2	1:A:273:SER:H	1.35	0.87
1:A:119:TRP:CZ3	1:A:150:ILE:HD11	2.10	0.87
1:A:232:LEU:HD23	1:A:245:VAL:HG11	1.55	0.87
1:A:230:LYS:N	1:A:230:LYS:HZ2	1.72	0.86
1:B:361:ALA:HB1	1:B:364:VAL:HB	1.57	0.86
1:D:347:LYS:HE3	1:D:347:LYS:H	1.38	0.86
1:A:119:TRP:HZ3	1:A:150:ILE:CD1	1.89	0.86
1:A:195:ALA:HB1	1:A:196:PRO:HD2	1.58	0.85
1:A:213:LYS:HD2	1:D:360:ILE:HD12	1.57	0.85
1:B:364:VAL:C	1:B:366:ALA:H	1.85	0.84
1:E:145:VAL:HG22	1:E:146:PRO:HD2	1.59	0.84
1:E:144:SER:O	1:E:145:VAL:CB	2.22	0.83
1:E:132:LYS:HD3	1:E:152:PHE:CE2	2.13	0.83
1:D:235:ASP:C	1:D:237:ASP:H	1.85	0.83
1:A:236:PRO:HA	1:A:239:VAL:HG23	1.59	0.83
1:A:195:ALA:CB	1:A:196:PRO:HD2	2.10	0.82
1:C:156:ASN:O	1:C:158:ARG:N	2.12	0.82
1:A:232:LEU:CD2	1:A:245:VAL:HG11	2.10	0.81
1:A:240:ALA:C	1:A:242:ASN:H	1.89	0.81
1:D:204:LEU:HA	1:D:208:GLN:NE2	1.95	0.81
1:E:122:ILE:HG12	1:E:161:PHE:CZ	2.15	0.81
1:A:230:LYS:HZ3	1:A:271:ASN:CG	1.89	0.81
1:A:164:GLU:OE2	1:A:164:GLU:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:VAL:CB	1:E:146:PRO:CD	2.59	0.80
1:B:336:THR:HG21	1:D:307:ARG:HH11	1.46	0.80
1:E:145:VAL:CG2	1:E:146:PRO:HD2	2.10	0.79
1:B:204:LEU:HA	1:B:208:GLN:HE21	1.44	0.79
1:C:158:ARG:HH22	1:C:207:GLU:CD	1.89	0.79
1:A:230:LYS:HE2	1:A:272:LEU:C	2.08	0.79
1:A:177:TYR:CE1	1:A:186:ARG:HG3	2.18	0.79
1:A:216:MET:HE1	1:A:259:ILE:HD12	1.64	0.79
1:A:276:ARG:HH21	1:A:276:ARG:HB3	1.48	0.78
1:A:230:LYS:CE	1:A:230:LYS:CA	2.61	0.78
1:A:230:LYS:CE	1:A:273:SER:N	2.46	0.76
1:E:145:VAL:CB	1:E:146:PRO:HD2	2.13	0.76
1:C:238:LEU:H	1:C:238:LEU:CD2	1.97	0.76
1:D:212:LEU:HG	1:D:216:MET:CE	2.16	0.75
1:D:235:ASP:HB3	1:D:236:PRO:CD	2.17	0.75
1:B:204:LEU:HA	1:B:208:GLN:HE22	1.52	0.75
1:C:212:LEU:HG	1:C:216:MET:CE	2.17	0.75
1:B:205:LYS:HG2	1:B:208:GLN:CD	2.12	0.75
1:B:238:LEU:CD2	1:B:245:VAL:HG21	2.17	0.74
1:C:158:ARG:NH2	1:C:207:GLU:OE2	2.19	0.74
1:A:204:LEU:HD22	1:A:208:GLN:NE2	2.02	0.74
1:B:327:LEU:O	1:B:330:THR:HB	1.87	0.74
1:A:230:LYS:NZ	1:A:271:ASN:C	2.45	0.74
1:D:219:ARG:NH2	1:D:235:ASP:OD2	2.20	0.74
1:D:235:ASP:O	1:D:237:ASP:OD1	2.06	0.74
1:A:288:GLN:HE22	1:B:287:VAL:HB	1.53	0.73
1:C:238:LEU:H	1:C:238:LEU:HD23	1.51	0.73
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.54	0.73
1:A:248:ASN:H	1:A:248:ASN:ND2	1.87	0.73
1:A:240:ALA:O	1:A:242:ASN:N	2.21	0.72
1:C:216:MET:HE1	1:C:259:ILE:HD12	1.71	0.72
1:A:306:GLU:H	1:A:306:GLU:CD	1.97	0.72
1:C:327:LEU:O	1:C:330:THR:HB	1.89	0.72
1:E:122:ILE:HG12	1:E:161:PHE:CE2	2.25	0.72
1:A:158:ARG:NH1	1:A:160:GLN:OE1	2.19	0.71
1:A:327:LEU:O	1:A:330:THR:HB	1.89	0.71
1:A:235:ASP:OD1	1:A:236:PRO:O	2.08	0.71
1:B:212:LEU:HG	1:B:216:MET:CE	2.20	0.71
1:B:216:MET:CE	1:B:259:ILE:HD12	2.20	0.71
1:A:240:ALA:C	1:A:242:ASN:N	2.45	0.71
1:B:366:ALA:CB	1:B:367:PRO:CD	2.62	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ARG:HH21	1:D:258:ARG:HG3	1.55	0.71
1:D:327:LEU:C	1:D:327:LEU:HD12	2.16	0.71
1:D:327:LEU:O	1:D:330:THR:HB	1.91	0.71
1:A:236:PRO:O	1:A:237:ASP:HB2	1.89	0.70
1:D:205:LYS:H	1:D:208:GLN:CD	1.99	0.70
1:A:165:ASP:OD2	1:A:165:ASP:C	2.21	0.70
1:D:235:ASP:CB	1:D:236:PRO:HD3	2.21	0.70
1:C:307:ARG:O	1:C:309:LEU:N	2.25	0.70
1:A:212:LEU:HG	1:A:216:MET:CE	2.22	0.70
1:A:230:LYS:HZ3	1:A:271:ASN:CB	2.03	0.70
1:B:365:GLU:OE1	1:B:365:GLU:HA	1.92	0.70
1:E:120:PHE:CE1	1:E:166:ALA:HA	2.26	0.70
1:C:304:LYS:HD3	1:C:326:SER:OG	1.92	0.69
1:C:319:GLU:HG3	1:C:350:ARG:HB2	1.74	0.69
1:C:237:ASP:O	1:C:238:LEU:C	2.35	0.69
1:D:347:LYS:H	1:D:347:LYS:CE	2.06	0.69
1:A:126:TYR:HA	1:A:157:THR:CG2	2.20	0.69
1:A:327:LEU:C	1:A:327:LEU:HD12	2.16	0.69
1:D:216:MET:CE	1:D:259:ILE:HD12	2.23	0.69
1:E:121:LYS:HB2	1:E:121:LYS:NZ	2.08	0.69
1:C:176:ASN:CG	1:C:177:TYR:HD1	2.00	0.68
1:D:349:LEU:HD13	1:E:132:LYS:HE3	1.73	0.68
1:C:147:PHE:CE1	1:C:149:PRO:HD3	2.29	0.68
1:A:230:LYS:HE2	1:A:272:LEU:CA	2.24	0.68
1:E:121:LYS:HG3	1:E:121:LYS:O	1.93	0.68
1:D:318:GLU:HB2	1:D:319:GLU:OE1	1.93	0.68
1:B:364:VAL:C	1:B:366:ALA:N	2.46	0.67
1:D:204:LEU:HD11	1:D:252:CYS:HA	1.76	0.67
1:A:249:ARG:HE	1:A:249:ARG:HA	1.59	0.67
1:B:232:LEU:HD23	1:B:245:VAL:HG11	1.76	0.67
1:D:219:ARG:HH11	1:D:232:LEU:CD1	2.07	0.67
1:A:216:MET:CE	1:A:259:ILE:HD12	2.25	0.66
1:B:365:GLU:OE1	1:B:365:GLU:CA	2.43	0.66
1:B:327:LEU:C	1:B:327:LEU:HD12	2.20	0.66
1:B:361:ALA:CB	1:B:364:VAL:HB	2.25	0.65
1:D:236:PRO:HB2	1:D:242:ASN:CG	2.20	0.65
1:A:205:LYS:HG2	1:A:208:GLN:OE1	1.96	0.65
1:C:327:LEU:HD12	1:C:327:LEU:C	2.20	0.65
1:B:305:SER:OG	1:B:307:ARG:HG2	1.96	0.65
1:B:204:LEU:HD11	1:B:252:CYS:SG	2.36	0.65
1:B:241:GLN:HE21	1:B:241:GLN:N	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:GLN:HG3	1:C:125:PRO:HB3	1.79	0.65
1:C:237:ASP:C	1:C:239:VAL:N	2.55	0.65
1:E:119:TRP:CZ3	1:E:150:ILE:HG21	2.31	0.65
1:C:119:TRP:CD2	1:C:164:GLU:HB3	2.32	0.64
1:A:230:LYS:NZ	1:A:230:LYS:N	2.45	0.64
1:C:331:PHE:HD2	1:C:336:THR:HG22	1.63	0.64
1:A:231:GLY:HA2	1:A:274:ASN:O	1.98	0.64
1:C:288:GLN:HE21	1:D:287:VAL:HB	1.63	0.64
1:C:237:ASP:HA	1:C:240:ALA:HB3	1.79	0.63
1:A:276:ARG:HB3	1:A:276:ARG:NH2	2.12	0.63
1:B:212:LEU:HG	1:B:216:MET:HE2	1.80	0.63
1:B:235:ASP:O	1:B:239:VAL:HG23	1.98	0.63
1:D:204:LEU:HA	1:D:208:GLN:HE22	1.61	0.63
1:C:147:PHE:CD1	1:C:149:PRO:HD3	2.34	0.63
1:D:245:VAL:HG12	1:D:245:VAL:O	1.99	0.62
1:D:273:SER:HB3	1:D:297:ASN:ND2	2.14	0.62
1:D:279:ARG:CB	1:D:279:ARG:HH11	2.12	0.62
1:B:205:LYS:H	1:B:208:GLN:NE2	1.97	0.62
1:A:294:LYS:HD3	1:A:318:GLU:OE1	1.99	0.62
1:D:205:LYS:HB2	1:D:208:GLN:HG3	1.82	0.62
1:C:211:GLN:O	1:C:215:ILE:HG13	2.00	0.62
1:C:215:ILE:HD13	1:C:238:LEU:HD22	1.82	0.62
1:D:232:LEU:O	1:D:236:PRO:HD2	2.00	0.62
1:A:205:LYS:H	1:A:208:GLN:CD	2.07	0.62
1:A:195:ALA:HB1	1:A:196:PRO:CD	2.28	0.62
1:B:365:GLU:OE1	1:B:365:GLU:O	2.19	0.61
1:E:150:ILE:HG23	1:E:162:PHE:HB2	1.81	0.61
1:A:238:LEU:HG	1:A:238:LEU:O	2.00	0.61
1:C:122:ILE:HD13	1:C:122:ILE:N	2.16	0.61
1:C:215:ILE:O	1:C:219:ARG:HG3	2.00	0.61
1:E:121:LYS:HB2	1:E:121:LYS:HZ2	1.65	0.61
1:A:273:SER:HB3	1:A:297:ASN:ND2	2.16	0.61
1:B:204:LEU:CA	1:B:208:GLN:NE2	2.58	0.61
1:A:142:LYS:HG3	1:A:179:ILE:HD11	1.82	0.61
1:E:153:HIS:NE2	1:E:160:GLN:NE2	2.49	0.61
1:A:147:PHE:CE1	1:A:149:PRO:HD3	2.35	0.61
1:A:236:PRO:HA	1:A:239:VAL:CG2	2.30	0.61
1:D:347:LYS:HE3	1:D:347:LYS:N	2.13	0.61
1:A:119:TRP:CZ3	1:A:150:ILE:CD1	2.76	0.60
1:E:122:ILE:HD12	1:E:123:THR:O	2.00	0.60
1:A:217:SER:HA	1:D:362:PHE:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLN:NE2	1:C:243:ILE:O	2.31	0.60
1:D:215:ILE:O	1:D:218:LYS:HG2	2.00	0.60
1:B:360:ILE:HB	1:C:213:LYS:HE2	1.82	0.60
1:C:288:GLN:NE2	1:D:287:VAL:HB	2.17	0.60
1:C:311:LYS:HE2	1:D:258:ARG:NH1	2.17	0.60
1:D:231:GLY:HA2	1:D:274:ASN:O	2.02	0.60
1:A:122:ILE:N	1:A:122:ILE:CD1	2.65	0.60
1:A:331:PHE:HD2	1:A:336:THR:HG22	1.66	0.60
1:C:273:SER:HB3	1:C:297:ASN:ND2	2.17	0.59
1:C:292:ASN:O	1:C:294:LYS:HG3	2.02	0.59
1:E:145:VAL:CG1	1:E:146:PRO:CD	2.59	0.59
1:C:271:ASN:ND2	1:C:273:SER:H	2.01	0.59
1:C:238:LEU:HD23	1:C:238:LEU:N	2.18	0.59
1:D:212:LEU:HG	1:D:216:MET:HE2	1.83	0.59
1:A:250:ARG:HG2	1:B:250:ARG:HD3	1.85	0.58
1:C:126:TYR:HA	1:C:157:THR:CG2	2.31	0.58
1:A:173:LYS:HB2	1:A:191:ILE:HD12	1.84	0.58
1:A:230:LYS:HG2	1:A:271:ASN:OD1	2.03	0.58
1:A:232:LEU:HD23	1:A:245:VAL:CG1	2.29	0.58
1:A:249:ARG:HA	1:A:249:ARG:NE	2.18	0.58
1:C:176:ASN:CG	1:C:177:TYR:CD1	2.79	0.58
1:C:287:VAL:HB	1:D:288:GLN:OE1	2.03	0.58
1:A:230:LYS:HD3	1:A:273:SER:O	2.02	0.58
1:B:271:ASN:C	1:B:271:ASN:HD22	2.10	0.58
1:B:237:ASP:HA	1:B:240:ALA:HB3	1.86	0.58
1:D:240:ALA:O	1:D:241:GLN:HG3	2.04	0.58
1:D:271:ASN:ND2	1:D:273:SER:H	2.01	0.58
1:E:173:LYS:HE3	1:E:173:LYS:HA	1.86	0.58
1:A:230:LYS:CE	1:A:273:SER:H	2.11	0.58
1:C:234:SER:HA	1:C:239:VAL:CG2	2.33	0.58
1:C:343:GLU:OE2	1:C:344:ARG:HD2	2.04	0.58
1:E:120:PHE:CZ	1:E:166:ALA:HA	2.39	0.58
1:A:205:LYS:N	1:A:208:GLN:OE1	2.30	0.57
1:B:271:ASN:ND2	1:B:273:SER:H	2.01	0.57
1:D:279:ARG:HH11	1:D:279:ARG:HB3	1.67	0.57
1:E:132:LYS:HG3	1:E:136:LEU:HG	1.86	0.57
1:D:279:ARG:HB3	1:D:279:ARG:NH1	2.19	0.57
1:A:230:LYS:HD2	1:A:273:SER:CB	2.32	0.57
1:D:331:PHE:HD2	1:D:336:THR:HG22	1.68	0.57
1:C:122:ILE:HD12	1:C:191:ILE:HG12	1.87	0.57
1:B:273:SER:HB3	1:B:297:ASN:ND2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ASN:C	1:C:271:ASN:HD22	2.12	0.57
1:A:230:LYS:HD2	1:A:271:ASN:HD21	1.70	0.57
1:B:366:ALA:H	1:B:367:PRO:HD2	1.70	0.56
1:C:142:LYS:HB3	1:C:175:VAL:HG13	1.87	0.56
1:C:164:GLU:OE2	1:C:164:GLU:C	2.48	0.56
1:A:147:PHE:CD1	1:A:149:PRO:HD3	2.40	0.56
1:D:358:PRO:HD3	1:E:149:PRO:HD3	1.87	0.56
1:C:212:LEU:HG	1:C:216:MET:HE2	1.87	0.56
1:C:216:MET:CE	1:C:259:ILE:HD12	2.35	0.56
1:A:230:LYS:HD2	1:A:271:ASN:ND2	2.20	0.56
1:B:342:ARG:NH1	1:B:348:LEU:O	2.39	0.56
1:C:119:TRP:CE3	1:C:164:GLU:HB3	2.40	0.56
1:D:242:ASN:C	1:D:243:ILE:O	2.42	0.56
1:B:332:ARG:NH1	1:D:304:LYS:HE3	2.22	0.55
1:B:304:LYS:HE2	1:D:332:ARG:NH1	2.21	0.55
1:C:212:LEU:HG	1:C:216:MET:HE3	1.89	0.55
1:C:313:LYS:HD2	1:C:313:LYS:O	2.06	0.55
1:A:211:GLN:HE21	1:E:145:VAL:HG11	1.71	0.55
1:C:331:PHE:CD2	1:C:336:THR:HG22	2.41	0.55
1:A:294:LYS:HE3	1:A:294:LYS:HA	1.87	0.55
1:A:328:CYS:C	1:A:330:THR:H	2.14	0.55
1:C:261:GLU:OE2	1:C:289:LYS:HE3	2.07	0.55
1:A:156:ASN:OD1	1:A:207:GLU:OE2	2.25	0.54
1:C:158:ARG:CZ	1:C:207:GLU:OE2	2.55	0.54
1:D:219:ARG:NH1	1:D:232:LEU:CD1	2.70	0.54
1:A:207:GLU:O	1:A:211:GLN:HG3	2.07	0.54
1:B:364:VAL:O	1:B:366:ALA:N	2.39	0.54
1:C:173:LYS:HB2	1:C:191:ILE:HD12	1.87	0.54
1:C:142:LYS:NZ	1:C:142:LYS:HA	2.22	0.54
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.07	0.54
1:C:158:ARG:NH1	1:C:207:GLU:OE2	2.41	0.54
1:A:244:ASP:O	1:A:246:VAL:HG23	2.07	0.54
1:A:238:LEU:CD2	1:A:243:ILE:O	2.47	0.54
1:A:319:GLU:HG3	1:A:350:ARG:HB2	1.90	0.54
1:C:142:LYS:HD3	1:C:178:LYS:CG	2.32	0.54
1:C:173:LYS:NZ	1:C:191:ILE:HB	2.23	0.54
1:E:122:ILE:HG21	1:E:172:LEU:HD13	1.90	0.54
1:A:136:LEU:HD22	1:A:149:PRO:HG2	1.90	0.54
1:B:238:LEU:HG	1:B:245:VAL:HG23	1.90	0.53
1:D:258:ARG:HG3	1:D:258:ARG:NH2	2.17	0.53
1:D:306:GLU:HG2	1:D:344:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PHE:CD2	1:A:336:THR:HG22	2.43	0.53
1:B:266:GLU:CD	1:B:266:GLU:H	2.16	0.53
1:B:205:LYS:N	1:B:208:GLN:NE2	2.55	0.53
1:A:128:ARG:HH11	1:A:128:ARG:CG	2.19	0.53
1:D:205:LYS:HD3	1:D:208:GLN:OE1	2.09	0.53
1:D:212:LEU:HG	1:D:216:MET:HE3	1.90	0.53
1:D:349:LEU:CD1	1:E:132:LYS:HE3	2.37	0.53
1:C:241:GLN:HG3	1:C:243:ILE:H	1.73	0.53
1:C:319:GLU:OE1	1:C:350:ARG:NH1	2.41	0.53
1:D:232:LEU:O	1:D:236:PRO:CD	2.57	0.53
1:D:305:SER:OG	1:D:307:ARG:HG2	2.09	0.53
1:C:271:ASN:HD22	1:C:272:LEU:N	2.06	0.52
1:B:331:PHE:HD2	1:B:336:THR:HG22	1.74	0.52
1:C:311:LYS:HE2	1:D:258:ARG:HH11	1.73	0.52
1:C:278:TYR:OH	1:C:279:ARG:NH1	2.42	0.52
1:D:219:ARG:NH1	1:D:232:LEU:HD12	2.24	0.52
1:B:323:ASP:CB	1:C:177:TYR:CE2	2.60	0.52
1:D:219:ARG:CZ	1:D:235:ASP:OD2	2.58	0.52
1:B:215:ILE:HD11	1:B:237:ASP:HB2	1.91	0.52
1:C:136:LEU:HD22	1:C:149:PRO:HG2	1.90	0.52
1:D:271:ASN:C	1:D:271:ASN:HD22	2.18	0.52
1:E:132:LYS:HD3	1:E:152:PHE:CD2	2.44	0.52
1:B:271:ASN:HD22	1:B:272:LEU:N	2.06	0.52
1:E:140:GLN:O	1:E:141:SER:C	2.51	0.52
1:B:236:PRO:O	1:B:239:VAL:N	2.42	0.52
1:B:324:GLY:CA	1:C:186:ARG:NH1	2.73	0.52
1:E:131:ASP:HB3	1:E:134:TRP:HB3	1.92	0.52
1:B:365:GLU:OE1	1:B:365:GLU:C	2.53	0.52
1:B:205:LYS:HG2	1:B:208:GLN:CG	2.40	0.51
1:D:342:ARG:NH1	1:D:348:LEU:O	2.44	0.51
1:A:347:LYS:NZ	1:A:347:LYS:HB3	2.25	0.51
1:A:248:ASN:H	1:A:248:ASN:HD22	1.57	0.51
1:A:338:ILE:HD13	1:A:356:LEU:HD22	1.93	0.51
1:A:271:ASN:C	1:A:271:ASN:HD22	2.19	0.51
1:D:331:PHE:CD2	1:D:336:THR:HG22	2.45	0.51
1:A:164:GLU:O	1:A:164:GLU:CD	2.53	0.51
1:A:271:ASN:HD22	1:A:272:LEU:N	2.09	0.51
1:B:231:GLY:HA2	1:B:274:ASN:O	2.11	0.51
1:A:172:LEU:HB3	1:A:191:ILE:HD11	1.92	0.50
1:C:340:ALA:O	1:C:343:GLU:HB3	2.10	0.50
1:A:142:LYS:HG3	1:A:179:ILE:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:LYS:HE3	1:D:258:ARG:CZ	2.42	0.50
1:D:243:ILE:HG22	1:D:244:ASP:N	2.26	0.50
1:A:212:LEU:HG	1:A:216:MET:HE3	1.92	0.50
1:A:212:LEU:HG	1:A:216:MET:HE2	1.92	0.50
1:B:205:LYS:HG2	1:B:208:GLN:HG3	1.92	0.50
1:A:165:ASP:OD2	1:A:166:ALA:N	2.45	0.50
1:A:230:LYS:HZ2	1:A:230:LYS:CA	2.23	0.50
1:B:232:LEU:CD2	1:B:245:VAL:HG11	2.41	0.50
1:A:218:LYS:NZ	1:A:218:LYS:HB3	2.27	0.50
1:D:234:SER:O	1:D:235:ASP:C	2.54	0.50
1:C:231:GLY:HA2	1:C:274:ASN:O	2.11	0.50
1:C:238:LEU:O	1:C:241:GLN:HG2	2.11	0.50
1:C:156:ASN:HD22	1:C:157:THR:H	1.60	0.50
1:D:338:ILE:HD13	1:D:356:LEU:HD22	1.93	0.50
1:B:238:LEU:CD2	1:B:245:VAL:CG2	2.87	0.50
1:D:213:LYS:HB2	1:D:213:LYS:NZ	2.27	0.50
1:A:219:ARG:NH1	1:A:232:LEU:HD12	2.26	0.49
1:A:271:ASN:ND2	1:A:273:SER:H	2.10	0.49
1:B:230:LYS:NZ	1:B:230:LYS:HB3	2.26	0.49
1:C:132:LYS:HE3	1:C:152:PHE:CD2	2.47	0.49
1:C:176:ASN:ND2	1:C:177:TYR:CD1	2.80	0.49
1:D:219:ARG:HH11	1:D:232:LEU:HD12	1.74	0.49
1:A:235:ASP:OD1	1:A:236:PRO:N	2.45	0.49
1:A:342:ARG:NH1	1:A:348:LEU:O	2.44	0.49
1:D:294:LYS:HG3	1:D:316:LYS:O	2.12	0.49
1:A:230:LYS:HZ3	1:A:271:ASN:HB3	1.76	0.49
1:B:295:ILE:HG12	1:B:319:GLU:HB3	1.94	0.49
1:D:271:ASN:HD22	1:D:272:LEU:N	2.09	0.49
1:D:293:LEU:O	1:D:294:LYS:HD2	2.12	0.49
1:A:196:PRO:HB2	1:A:199:THR:OG1	2.12	0.49
1:A:204:LEU:CD2	1:A:208:GLN:NE2	2.74	0.49
1:B:323:ASP:CA	1:C:177:TYR:HE2	2.23	0.49
1:B:331:PHE:CD2	1:B:336:THR:HG22	2.48	0.49
1:C:338:ILE:HD13	1:C:356:LEU:HD22	1.95	0.49
1:E:151:GLU:HG3	1:E:153:HIS:HD1	1.77	0.49
1:A:210:GLU:HG3	1:D:360:ILE:HD11	1.95	0.49
1:B:241:GLN:N	1:B:241:GLN:NE2	2.61	0.49
1:C:311:LYS:CE	1:D:258:ARG:NH1	2.76	0.49
1:A:243:ILE:N	1:A:243:ILE:HD12	2.28	0.48
1:B:289:LYS:C	1:B:291:PRO:HD3	2.38	0.48
1:D:351:LEU:O	1:D:352:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LYS:C	1:C:291:PRO:HD3	2.39	0.48
1:C:225:GLN:HG2	1:C:266:GLU:OE2	2.14	0.48
1:C:142:LYS:HA	1:C:142:LYS:HZ3	1.78	0.48
1:D:207:GLU:OE2	1:D:208:GLN:HG3	2.13	0.48
1:B:364:VAL:HG22	1:B:367:PRO:CB	2.34	0.48
1:D:235:ASP:CB	1:D:236:PRO:CD	2.83	0.48
1:D:239:VAL:C	1:D:241:GLN:N	2.71	0.48
1:B:294:LYS:HG3	1:B:295:ILE:HG13	1.94	0.48
1:C:197:PRO:C	1:C:198:HIS:CG	2.92	0.48
1:C:258:ARG:CZ	1:D:311:LYS:HE3	2.43	0.48
1:D:242:ASN:O	1:D:243:ILE:C	2.56	0.48
1:A:142:LYS:HB2	1:A:175:VAL:HG13	1.96	0.48
1:A:248:ASN:ND2	1:A:248:ASN:N	2.57	0.48
1:B:215:ILE:CG1	1:B:238:LEU:HD13	2.28	0.48
1:C:237:ASP:O	1:C:239:VAL:C	2.57	0.48
1:D:266:GLU:H	1:D:266:GLU:CD	2.22	0.48
1:E:122:ILE:HD12	1:E:123:THR:N	2.29	0.48
1:A:358:PRO:HA	1:A:359:PRO:HD3	1.82	0.48
1:B:271:ASN:C	1:B:271:ASN:ND2	2.71	0.47
1:C:176:ASN:OD1	1:C:177:TYR:CD1	2.67	0.47
1:D:327:LEU:HD12	1:D:328:CYS:N	2.29	0.47
1:C:172:LEU:HD12	1:C:172:LEU:HA	1.67	0.47
1:D:205:LYS:HB2	1:D:208:GLN:CG	2.44	0.47
1:D:327:LEU:C	1:D:327:LEU:CD1	2.87	0.47
1:A:140:GLN:OE1	1:A:146:PRO:HA	2.14	0.47
1:D:204:LEU:HD23	1:D:208:GLN:NE2	2.29	0.47
1:B:324:GLY:HA3	1:C:186:ARG:NH1	2.28	0.47
1:C:119:TRP:CD1	1:C:196:PRO:HG3	2.49	0.47
1:A:263:ASN:HB3	1:D:362:PHE:CD1	2.49	0.47
1:B:226:VAL:HG13	1:B:269:SER:HB3	1.96	0.47
1:C:156:ASN:ND2	1:C:157:THR:N	2.63	0.47
1:D:358:PRO:HA	1:D:359:PRO:HD3	1.82	0.47
1:A:132:LYS:HE3	1:A:152:PHE:CD2	2.49	0.47
1:A:230:LYS:CD	1:A:271:ASN:ND2	2.78	0.47
1:C:342:ARG:NH1	1:C:348:LEU:O	2.48	0.47
1:D:238:LEU:C	1:D:238:LEU:HD13	2.39	0.47
1:E:134:TRP:O	1:E:138:MET:HB2	2.14	0.47
1:A:250:ARG:HD3	1:B:250:ARG:HG2	1.97	0.47
1:C:258:ARG:NE	1:D:311:LYS:HE3	2.30	0.47
1:A:230:LYS:HG2	1:A:271:ASN:CG	2.40	0.47
1:A:249:ARG:HH11	1:A:279:ARG:NH2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LEU:CD2	1:C:245:VAL:HG11	2.44	0.47
1:D:204:LEU:HD23	1:D:208:GLN:HE21	1.80	0.47
1:B:236:PRO:HB2	1:B:237:ASP:OD1	2.13	0.46
1:A:180:LEU:HD21	1:A:184:ASN:OD1	2.14	0.46
1:B:364:VAL:HA	1:B:367:PRO:HD2	1.97	0.46
1:C:307:ARG:O	1:C:308:GLU:C	2.57	0.46
1:A:118:ASN:OD1	1:A:118:ASN:N	2.48	0.46
1:A:236:PRO:O	1:A:237:ASP:CB	2.60	0.46
1:A:305:SER:OG	1:A:306:GLU:N	2.48	0.46
1:D:219:ARG:HH11	1:D:232:LEU:HD13	1.77	0.46
1:C:122:ILE:N	1:C:122:ILE:CD1	2.78	0.46
1:A:122:ILE:N	1:A:122:ILE:HD13	2.31	0.46
1:D:244:ASP:HB3	1:D:246:VAL:HG23	1.97	0.46
1:E:137:SER:O	1:E:141:SER:N	2.40	0.46
1:B:336:THR:HG21	1:D:307:ARG:NH1	2.25	0.46
1:C:271:ASN:ND2	1:C:271:ASN:C	2.72	0.46
1:A:289:LYS:C	1:A:291:PRO:HD3	2.41	0.46
1:D:204:LEU:CD1	1:D:252:CYS:HA	2.44	0.46
1:D:289:LYS:C	1:D:291:PRO:HD3	2.40	0.46
1:E:145:VAL:HG13	1:E:146:PRO:N	2.26	0.46
1:B:246:VAL:O	1:B:249:ARG:HB2	2.16	0.45
1:A:258:ARG:CZ	1:B:311:LYS:HE3	2.46	0.45
1:D:264:ILE:N	1:D:265:PRO:HD3	2.32	0.45
1:D:273:SER:HB3	1:D:297:ASN:HD22	1.80	0.45
1:D:309:LEU:HD11	1:D:322:LEU:HD11	1.98	0.45
1:C:232:LEU:HD23	1:C:245:VAL:HG11	1.99	0.45
1:A:233:ARG:HG2	1:A:244:ASP:OD1	2.16	0.45
1:C:156:ASN:HD22	1:C:157:THR:N	2.14	0.45
1:A:176:ASN:OD1	1:A:188:SER:HA	2.16	0.45
1:A:288:GLN:H	1:A:288:GLN:HG2	1.52	0.45
1:A:327:LEU:HD12	1:A:328:CYS:N	2.32	0.45
1:B:204:LEU:HD12	1:B:204:LEU:N	2.32	0.45
1:B:363:ASP:C	1:B:365:GLU:N	2.74	0.45
1:B:257:LEU:HD11	1:B:283:MET:HA	1.99	0.45
1:B:309:LEU:HD11	1:B:322:LEU:HD11	1.98	0.45
1:E:144:SER:O	1:E:145:VAL:HB	2.14	0.45
1:C:219:ARG:NH1	1:C:232:LEU:HD12	2.32	0.44
1:A:155:GLU:OE2	1:A:205:LYS:CE	2.66	0.44
1:E:140:GLN:C	1:E:142:LYS:N	2.75	0.44
1:C:264:ILE:N	1:C:265:PRO:HD3	2.32	0.44
1:B:324:GLY:CA	1:C:186:ARG:HH12	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:GLU:OE1	1:C:207:GLU:N	2.50	0.44
1:D:205:LYS:HB2	1:D:208:GLN:OE1	2.18	0.44
1:D:271:ASN:ND2	1:D:271:ASN:C	2.76	0.44
1:A:182:ARG:HG2	1:A:183:GLU:N	2.32	0.44
1:B:251:SER:O	1:B:254:ALA:HB3	2.17	0.44
1:E:121:LYS:HZ1	1:E:160:GLN:HG2	1.83	0.44
1:B:213:LYS:HD2	1:B:213:LYS:C	2.42	0.44
1:C:176:ASN:OD1	1:C:188:SER:HA	2.18	0.44
1:E:153:HIS:HE1	1:E:162:PHE:HE1	1.64	0.44
1:A:230:LYS:HE2	1:A:272:LEU:N	2.32	0.44
1:A:240:ALA:O	1:A:241:GLN:C	2.61	0.44
1:D:205:LYS:HB2	1:D:208:GLN:CD	2.43	0.44
1:B:246:VAL:HB	1:B:249:ARG:HH11	1.83	0.43
1:B:289:LYS:O	1:B:291:PRO:HD3	2.17	0.43
1:A:230:LYS:NZ	1:A:230:LYS:CA	2.80	0.43
1:B:351:LEU:O	1:B:352:ASP:HB2	2.17	0.43
1:C:309:LEU:HD11	1:C:322:LEU:HD11	2.00	0.43
1:A:204:LEU:HD12	1:A:255:ALA:CB	2.49	0.43
1:D:251:SER:O	1:D:254:ALA:HB3	2.18	0.43
1:D:294:LYS:HE3	1:D:316:LYS:HB2	2.00	0.43
1:A:214:LEU:HD23	1:E:146:PRO:HD3	2.00	0.43
1:A:332:ARG:NH2	1:A:332:ARG:HB2	2.33	0.43
1:A:128:ARG:CG	1:A:128:ARG:NH1	2.81	0.43
1:A:328:CYS:C	1:A:330:THR:N	2.77	0.43
1:B:366:ALA:N	1:B:367:PRO:HD2	2.33	0.43
1:D:213:LYS:HB2	1:D:213:LYS:HZ2	1.84	0.43
1:D:340:ALA:O	1:D:343:GLU:HB3	2.19	0.43
1:A:158:ARG:HD2	1:A:160:GLN:OE1	2.19	0.43
1:A:329:ASP:OD2	1:A:329:ASP:N	2.51	0.43
1:B:264:ILE:N	1:B:265:PRO:HD3	2.34	0.43
1:C:127:GLY:C	1:C:129:LYS:H	2.27	0.43
1:C:327:LEU:HD12	1:C:328:CYS:N	2.33	0.43
1:A:351:LEU:O	1:A:352:ASP:HB2	2.19	0.43
1:C:155:GLU:O	1:C:156:ASN:HB3	2.19	0.43
1:E:172:LEU:HD23	1:E:172:LEU:HA	1.89	0.43
1:A:264:ILE:N	1:A:265:PRO:HD3	2.34	0.42
1:A:128:ARG:NH1	1:A:154:TYR:CD1	2.86	0.42
1:A:331:PHE:HD2	1:A:336:THR:CG2	2.32	0.42
1:A:340:ALA:O	1:A:343:GLU:HB3	2.20	0.42
1:B:364:VAL:C	1:B:367:PRO:HD2	2.44	0.42
1:E:136:LEU:HD13	1:E:149:PRO:HG2	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:SER:HB3	1:A:297:ASN:HD22	1.84	0.42
1:A:279:ARG:HG3	1:A:279:ARG:O	2.18	0.42
1:C:131:ASP:HB3	1:C:134:TRP:HB3	2.01	0.42
1:C:156:ASN:ND2	1:C:157:THR:H	2.17	0.42
1:C:214:LEU:HG	1:C:218:LYS:HE3	2.01	0.42
1:D:239:VAL:C	1:D:241:GLN:H	2.27	0.42
1:A:150:ILE:O	1:A:150:ILE:HG13	2.20	0.42
1:A:230:LYS:CE	1:A:271:ASN:ND2	2.82	0.42
1:B:232:LEU:HD23	1:B:245:VAL:CG1	2.48	0.42
1:D:215:ILE:HA	1:D:218:LYS:HE3	2.02	0.42
1:D:317:LEU:N	1:D:347:LYS:NZ	2.67	0.42
1:C:128:ARG:O	1:C:128:ARG:HG3	2.19	0.42
1:B:327:LEU:HD12	1:B:328:CYS:N	2.34	0.42
1:B:338:ILE:HD13	1:B:356:LEU:HD22	2.00	0.42
1:C:180:LEU:HD21	1:C:184:ASN:OD1	2.19	0.42
1:D:219:ARG:NH1	1:D:232:LEU:HD13	2.34	0.42
1:A:216:MET:HG2	1:A:229:LEU:HD21	2.01	0.42
1:C:268:LEU:O	1:C:293:LEU:HD12	2.20	0.42
1:C:331:PHE:HD2	1:C:336:THR:CG2	2.29	0.42
1:D:205:LYS:N	1:D:208:GLN:CD	2.73	0.42
1:D:328:CYS:C	1:D:330:THR:H	2.26	0.42
1:A:175:VAL:HG12	1:A:175:VAL:O	2.20	0.42
1:D:224:GLN:HA	1:D:224:GLN:OE1	2.20	0.42
1:B:323:ASP:CA	1:C:177:TYR:CE2	3.02	0.42
1:C:150:ILE:O	1:C:150:ILE:HG13	2.19	0.42
1:D:295:ILE:HG12	1:D:319:GLU:CD	2.45	0.42
1:A:288:GLN:NE2	1:B:287:VAL:HB	2.29	0.41
1:A:289:LYS:O	1:A:291:PRO:HD3	2.20	0.41
1:B:204:LEU:CA	1:B:208:GLN:HE21	2.23	0.41
1:B:279:ARG:O	1:B:279:ARG:HG3	2.19	0.41
1:C:289:LYS:O	1:C:291:PRO:HD3	2.20	0.41
1:A:292:ASN:O	1:A:294:LYS:HG2	2.20	0.41
1:B:364:VAL:O	1:B:364:VAL:HG13	2.20	0.41
1:C:176:ASN:ND2	1:C:177:TYR:HD1	2.14	0.41
1:A:182:ARG:HG2	1:A:183:GLU:H	1.85	0.41
1:B:216:MET:HG2	1:B:229:LEU:HD21	2.03	0.41
1:B:365:GLU:O	1:B:365:GLU:CD	2.63	0.41
1:D:239:VAL:O	1:D:241:GLN:N	2.54	0.41
1:C:235:ASP:HB3	1:C:236:PRO:HD2	2.02	0.41
1:B:236:PRO:O	1:B:239:VAL:HB	2.20	0.41
1:B:246:VAL:HB	1:B:249:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:C	1:B:327:LEU:CD1	2.92	0.41
1:C:273:SER:HB3	1:C:297:ASN:HD22	1.86	0.41
1:D:355:GLU:OE1	1:D:355:GLU:N	2.53	0.41
1:A:229:LEU:C	1:A:230:LYS:NZ	2.79	0.41
1:C:175:VAL:HG12	1:C:175:VAL:O	2.20	0.41
1:D:347:LYS:H	1:D:347:LYS:CD	2.34	0.41
1:E:119:TRP:CE2	1:E:164:GLU:HB2	2.56	0.41
1:C:257:LEU:HD11	1:C:283:MET:HA	2.03	0.41
1:A:131:ASP:HB3	1:A:134:TRP:HB3	2.03	0.41
1:A:251:SER:O	1:A:254:ALA:HB3	2.21	0.41
1:A:287:VAL:HB	1:B:288:GLN:NE2	2.36	0.41
1:A:309:LEU:HD11	1:A:322:LEU:HD11	2.03	0.41
1:A:356:LEU:HA	1:A:357:PRO:HD3	1.93	0.41
1:B:358:PRO:HA	1:B:359:PRO:HD3	1.79	0.41
1:C:151:GLU:HB3	1:C:162:PHE:HD1	1.86	0.41
1:C:337:TYR:CE2	1:C:351:LEU:HD21	2.56	0.41
1:D:232:LEU:CD2	1:D:245:VAL:HG11	2.50	0.41
1:C:355:GLU:N	1:C:355:GLU:OE1	2.53	0.41
1:E:132:LYS:HD3	1:E:152:PHE:CZ	2.54	0.40
1:A:214:LEU:O	1:A:217:SER:OG	2.38	0.40
1:C:279:ARG:O	1:C:279:ARG:HG2	2.20	0.40
1:D:289:LYS:O	1:D:291:PRO:HD3	2.21	0.40
1:A:155:GLU:OE2	1:A:205:LYS:HE3	2.21	0.40
1:A:226:VAL:HG13	1:A:269:SER:HB3	2.03	0.40
1:C:241:GLN:HG3	1:C:243:ILE:N	2.36	0.40
1:A:204:LEU:HD12	1:A:255:ALA:HB2	2.03	0.40
1:B:324:GLY:HA3	1:C:186:ARG:HH12	1.86	0.40
1:C:176:ASN:O	1:C:177:TYR:HB2	2.21	0.40
1:D:216:MET:HG2	1:D:229:LEU:HD21	2.04	0.40
1:A:236:PRO:CA	1:A:239:VAL:HG23	2.42	0.40
1:A:271:ASN:C	1:A:271:ASN:ND2	2.79	0.40
1:B:334:GLN:O	1:B:335:SER:C	2.63	0.40
1:D:257:LEU:HD11	1:D:283:MET:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:LYS:NZ	1:E:142:LYS:NZ[8_665]	1.44	0.76

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	238/271 (88%)	213 (90%)	20 (8%)	5 (2%)	5	26
1	B	163/271 (60%)	149 (91%)	10 (6%)	4 (2%)	4	22
1	C	240/271 (89%)	216 (90%)	17 (7%)	7 (3%)	3	20
1	D	160/271 (59%)	139 (87%)	16 (10%)	5 (3%)	3	18
1	E	38/271 (14%)	35 (92%)	2 (5%)	1 (3%)	4	21
All	All	839/1355 (62%)	752 (90%)	65 (8%)	22 (3%)	4	21

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	PRO
1	C	157	THR
1	C	236	PRO
1	C	238	LEU
1	C	308	GLU
1	D	236	PRO
1	D	238	LEU
1	A	241	GLN
1	A	245	VAL
1	D	235	ASP
1	E	146	PRO
1	B	363	ASP
1	B	365	GLU
1	C	237	ASP
1	C	242	ASN
1	A	156	ASN
1	B	206	PRO
1	D	206	PRO
1	D	231	GLY
1	C	149	PRO
1	A	149	PRO

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Mol	Chain	Res	Type
1	A	195	ALA

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	222/245 (91%)	201 (90%)	21 (10%)	8	29
1	B	152/245 (62%)	142 (93%)	10 (7%)	15	42
1	C	222/245 (91%)	207 (93%)	15 (7%)	14	41
1	D	150/245 (61%)	141 (94%)	9 (6%)	17	45
1	E	39/245 (16%)	32 (82%)	7 (18%)	2	8
All	All	785/1225 (64%)	723 (92%)	62 (8%)	11	36

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ILE
1	A	128	ARG
1	A	149	PRO
1	A	172	LEU
1	A	181	ASP
1	A	182	ARG
1	A	197	PRO
1	A	198	HIS
1	A	206	PRO
1	A	213	LYS
1	A	230	LYS
1	A	248	ASN
1	A	288	GLN
1	A	294	LYS
1	A	297	ASN
1	A	306	GLU
1	A	329	ASP
1	A	330	THR

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Mol	Chain	Res	Type
1	A	339	SER
1	A	347	LYS
1	A	355	GLU
1	B	206	PRO
1	B	211	GLN
1	B	230	LYS
1	B	237	ASP
1	B	241	GLN
1	B	288	GLN
1	B	297	ASN
1	B	364	VAL
1	B	365	GLU
1	B	367	PRO
1	C	122	ILE
1	C	140	GLN
1	C	142	LYS
1	C	149	PRO
1	C	165	ASP
1	C	172	LEU
1	C	181	ASP
1	C	228	ASP
1	C	236	PRO
1	C	238	LEU
1	C	266	GLU
1	C	297	ASN
1	C	306	GLU
1	C	346	PRO
1	C	355	GLU
1	D	206	PRO
1	D	210	GLU
1	D	213	LYS
1	D	236	PRO
1	D	258	ARG
1	D	266	GLU
1	D	306	GLU
1	D	347	LYS
1	D	355	GLU
1	E	121	LYS
1	E	122	ILE
1	E	139	ILE
1	E	145	VAL
1	E	150	ILE

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Mol	Chain	Res	Type
1	E	164	GLU
1	E	173	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	156	ASN
1	A	248	ASN
1	A	271	ASN
1	A	274	ASN
1	A	288	GLN
1	A	292	ASN
1	A	297	ASN
1	B	208	GLN
1	B	211	GLN
1	B	241	GLN
1	B	271	ASN
1	B	274	ASN
1	B	297	ASN
1	C	156	ASN
1	C	271	ASN
1	C	297	ASN
1	C	334	GLN
1	D	208	GLN
1	D	271	ASN
1	E	160	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	242/271 (89%)	1.37	56 (23%)	2	2	55, 66, 89, 109	0
1	B	165/271 (60%)	1.32	37 (22%)	2	2	49, 63, 82, 97	0
1	C	244/271 (90%)	1.62	79 (32%)	1	1	55, 74, 106, 106	0
1	D	162/271 (59%)	1.46	46 (28%)	1	1	52, 65, 85, 100	0
1	E	44/271 (16%)	2.23	21 (47%)	0	1	89, 94, 94, 94	0
All	All	857/1355 (63%)	1.49	239 (27%)	1	1	49, 68, 106, 109	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	319	GLU	7.7
1	A	211	GLN	6.0
1	B	210	GLU	5.7
1	B	318	GLU	5.4
1	C	228	ASP	5.1
1	A	242	ASN	5.1
1	C	329	ASP	5.1
1	D	355	GLU	5.0
1	A	240	ALA	4.9
1	C	178	LYS	4.7
1	E	141	SER	4.7
1	C	266	GLU	4.7
1	C	183	GLU	4.7
1	B	365	GLU	4.6
1	B	207	GLU	4.6
1	B	360	ILE	4.5
1	A	318	GLU	4.5
1	B	363	ASP	4.5
1	B	362	PHE	4.5
1	B	359	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLU	4.3
1	E	139	ILE	4.3
1	B	203	GLU	4.2
1	C	242	ASN	4.2
1	E	138	MET	4.2
1	B	358	PRO	4.1
1	C	151	GLU	4.1
1	C	310	ASP	4.1
1	C	131	ASP	4.0
1	C	193	SER	4.0
1	D	244	ASP	4.0
1	D	362	PHE	3.9
1	E	136	LEU	3.9
1	D	242	ASN	3.9
1	C	165	ASP	3.9
1	E	143	CYS	3.9
1	B	244	ASP	3.9
1	C	188	SER	3.9
1	D	354	HIS	3.9
1	C	355	GLU	3.8
1	C	144	SER	3.8
1	D	210	GLU	3.8
1	A	323	ASP	3.8
1	D	239	VAL	3.8
1	C	146	PRO	3.8
1	A	294	LYS	3.8
1	D	238	LEU	3.8
1	D	365	GLU	3.7
1	E	140	GLN	3.7
1	B	366	ALA	3.7
1	B	319	GLU	3.7
1	D	262	GLU	3.7
1	D	363	ASP	3.6
1	C	142	LYS	3.6
1	A	235	ASP	3.6
1	E	149	PRO	3.6
1	A	249	ARG	3.6
1	E	164	GLU	3.6
1	E	153	HIS	3.5
1	A	279	ARG	3.5
1	D	334	GLN	3.5
1	C	173	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	282	ASP	3.5
1	D	347	LYS	3.5
1	D	235	ASP	3.5
1	D	237	ASP	3.4
1	B	367	PRO	3.4
1	D	359	PRO	3.4
1	B	364	VAL	3.4
1	C	157	THR	3.4
1	A	177	TYR	3.4
1	C	126	TYR	3.4
1	A	245	VAL	3.3
1	D	358	PRO	3.3
1	D	361	ALA	3.3
1	C	198	HIS	3.3
1	A	362	PHE	3.3
1	E	145	VAL	3.3
1	D	302	GLU	3.3
1	C	330	THR	3.3
1	D	211	GLN	3.3
1	C	141	SER	3.3
1	A	198	HIS	3.2
1	A	230	LYS	3.2
1	E	152	PHE	3.2
1	A	155	GLU	3.2
1	A	302	GLU	3.1
1	A	118	ASN	3.1
1	D	243	ILE	3.1
1	C	243	ILE	3.1
1	C	119	TRP	3.1
1	A	236	PRO	3.1
1	B	266	GLU	3.1
1	B	343	GLU	3.1
1	A	203	GLU	3.0
1	A	343	GLU	3.0
1	A	361	ALA	3.0
1	C	163	VAL	3.0
1	E	131	ASP	3.0
1	B	355	GLU	3.0
1	B	205	LYS	2.9
1	B	238	LEU	2.9
1	C	129	LYS	2.9
1	C	164	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	333	ASP	2.9
1	C	238	LEU	2.9
1	B	357	PRO	2.9
1	E	142	LYS	2.9
1	A	193	SER	2.9
1	C	140	GLN	2.9
1	D	346	PRO	2.9
1	A	359	PRO	2.8
1	C	236	PRO	2.8
1	A	241	GLN	2.8
1	C	326	SER	2.8
1	D	357	PRO	2.8
1	C	128	ARG	2.8
1	E	175	VAL	2.8
1	D	360	ILE	2.8
1	E	144	SER	2.8
1	A	332	ARG	2.8
1	D	236	PRO	2.8
1	A	239	VAL	2.8
1	E	171	ALA	2.8
1	A	306	GLU	2.8
1	A	216	MET	2.7
1	D	352	ASP	2.7
1	A	360	ILE	2.7
1	C	161	PHE	2.7
1	D	324	GLY	2.7
1	C	244	ASP	2.7
1	C	120	PHE	2.7
1	D	336	THR	2.7
1	C	177	TYR	2.7
1	A	179	ILE	2.7
1	D	207	GLU	2.7
1	A	119	TRP	2.7
1	B	294	LYS	2.7
1	B	361	ALA	2.7
1	C	267	LEU	2.7
1	A	210	GLU	2.7
1	C	252	CYS	2.7
1	A	265	PRO	2.6
1	C	334	GLN	2.6
1	E	134	TRP	2.6
1	C	323	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	196	PRO	2.6
1	C	249	ARG	2.6
1	C	241	GLN	2.6
1	B	335	SER	2.6
1	B	241	GLN	2.6
1	D	323	ASP	2.6
1	D	364	VAL	2.6
1	C	362	PHE	2.6
1	A	237	ASP	2.6
1	A	330	THR	2.6
1	B	316	LYS	2.6
1	C	182	ARG	2.6
1	E	160	GLN	2.5
1	B	239	VAL	2.5
1	A	164	GLU	2.5
1	C	210	GLU	2.5
1	B	204	LEU	2.5
1	C	194	SER	2.5
1	B	356	LEU	2.5
1	A	266	GLU	2.5
1	C	313	LYS	2.5
1	C	197	PRO	2.5
1	C	162	PHE	2.4
1	A	207	GLU	2.4
1	C	343	GLU	2.4
1	C	118	ASN	2.4
1	A	197	PRO	2.4
1	C	361	ALA	2.4
1	D	241	GLN	2.4
1	A	218	LYS	2.4
1	D	204	LEU	2.4
1	A	244	ASP	2.4
1	A	150	ILE	2.4
1	C	169	ALA	2.4
1	E	173	LYS	2.4
1	D	288	GLN	2.3
1	B	334	GLN	2.3
1	A	199	THR	2.3
1	D	332	ARG	2.3
1	B	206	PRO	2.3
1	B	288	GLN	2.3
1	C	186	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	307	ARG	2.3
1	D	356	LEU	2.3
1	C	179	ILE	2.2
1	C	148	THR	2.2
1	C	130	TYR	2.2
1	C	160	GLN	2.2
1	A	264	ILE	2.2
1	C	134	TRP	2.2
1	D	330	THR	2.2
1	A	156	ASN	2.2
1	C	207	GLU	2.2
1	D	240	ALA	2.2
1	C	149	PRO	2.2
1	C	167	SER	2.2
1	E	151	GLU	2.2
1	A	205	LYS	2.2
1	B	213	LYS	2.2
1	B	235	ASP	2.2
1	C	174	ALA	2.1
1	C	206	PRO	2.1
1	C	143	CYS	2.1
1	C	170	SER	2.1
1	D	318	GLU	2.1
1	A	281	ASP	2.1
1	C	122	ILE	2.1
1	D	295	ILE	2.1
1	B	302	GLU	2.1
1	B	246	VAL	2.1
1	A	347	LYS	2.1
1	C	288	GLN	2.1
1	C	125	PRO	2.1
1	A	305	SER	2.1
1	C	226	VAL	2.1
1	D	245	VAL	2.1
1	C	117	LYS	2.1
1	D	230	LYS	2.1
1	A	212	LEU	2.1
1	C	268	LEU	2.1
1	C	235	ASP	2.1
1	C	187	ILE	2.0
1	C	216	MET	2.0
1	C	159	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	352	ASP	2.0
1	A	151	GLU	2.0
1	D	218	LYS	2.0
1	C	145	VAL	2.0
1	E	123	THR	2.0
1	B	282	ASP	2.0
1	C	265	PRO	2.0
1	A	238	LEU	2.0
1	A	317	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.