



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2016 – 02:53 PM EDT

PDB ID : 5KNN
Title : Evolutionary gain of alanine mischarging to non-cognate tRNAs with a G4:U69 base pair
Authors : Sun, L.; He, W.; Yang, X.-L.
Deposited on : 2016-06-28
Resolution : 2.68 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

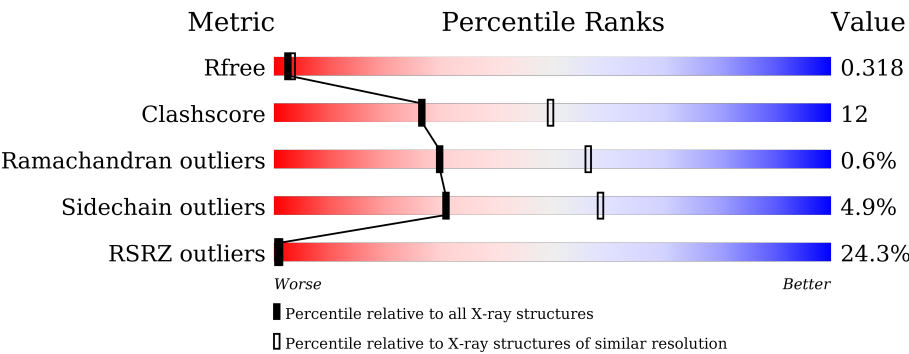
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	450	<div><div>18%</div><div><div></div><div>78%</div><div>19%</div><div>.</div></div></div>
1	B	450	<div><div>23%</div><div><div></div><div>73%</div><div>22%</div><div>..</div></div></div>
1	C	450	<div><div>28%</div><div><div></div><div>66%</div><div>26%</div><div>5%</div><div>..</div></div></div>
1	D	450	<div><div>29%</div><div><div></div><div>72%</div><div>23%</div><div>..</div></div></div>
1	E	450	<div><div>19%</div><div><div></div><div>74%</div><div>22%</div><div>..</div></div></div>
1	F	450	<div><div>20%</div><div><div></div><div>74%</div><div>23%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	450	<div><div></div><div>27%</div><div></div><div>73%</div><div></div><div>24%</div><div></div><div>• •</div></div>
1	H	450	<div><div></div><div>29%</div><div></div><div>69%</div><div></div><div>25%</div><div></div><div>• ••</div></div>

2 Entry composition

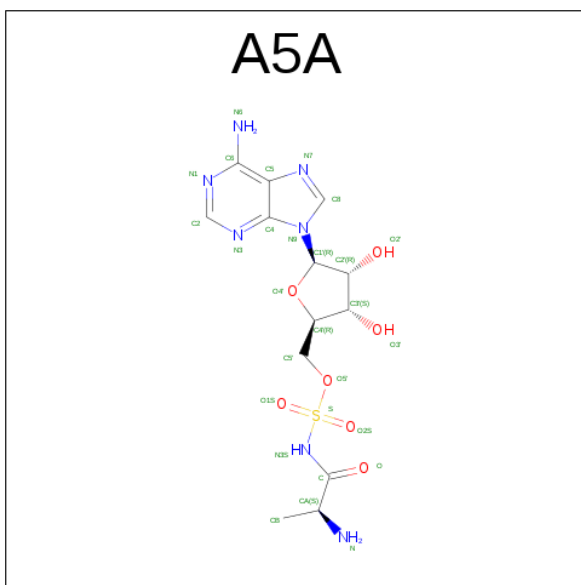
There are 2 unique types of molecules in this entry. The entry contains 28584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alanine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	B	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	C	444	Total	C	N	O	S	0	0	0
			3514	2227	604	667	16			
1	D	447	Total	C	N	O	S	0	0	0
			3536	2241	608	671	16			
1	E	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	F	449	Total	C	N	O	S	0	0	0
			3551	2250	611	674	16			
1	G	449	Total	C	N	O	S	0	0	0
			3551	2250	611	674	16			
1	H	446	Total	C	N	O	S	0	0	0
			3528	2235	607	670	16			

- Molecule 2 is '5'-O-(N-(L-ALANYL)-SULFAMOYL)ADENOSINE (three-letter code: A5A) (formula: C₁₃H₁₉N₇O₇S).

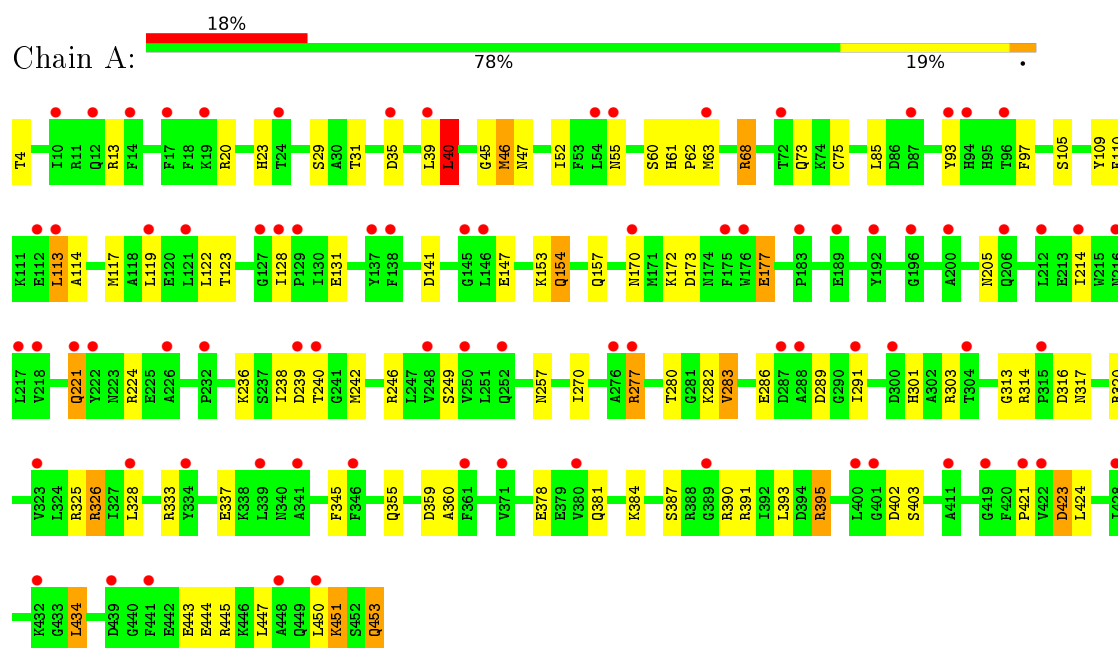


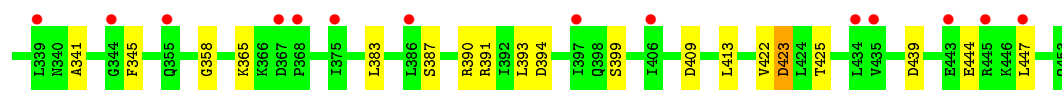
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	B	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	C	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	D	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	E	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	F	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	G	1	Total 28	C 13	N 7	O 7	S 1	0	0
2	H	1	Total 28	C 13	N 7	O 7	S 1	0	0

3 Residue-property plots

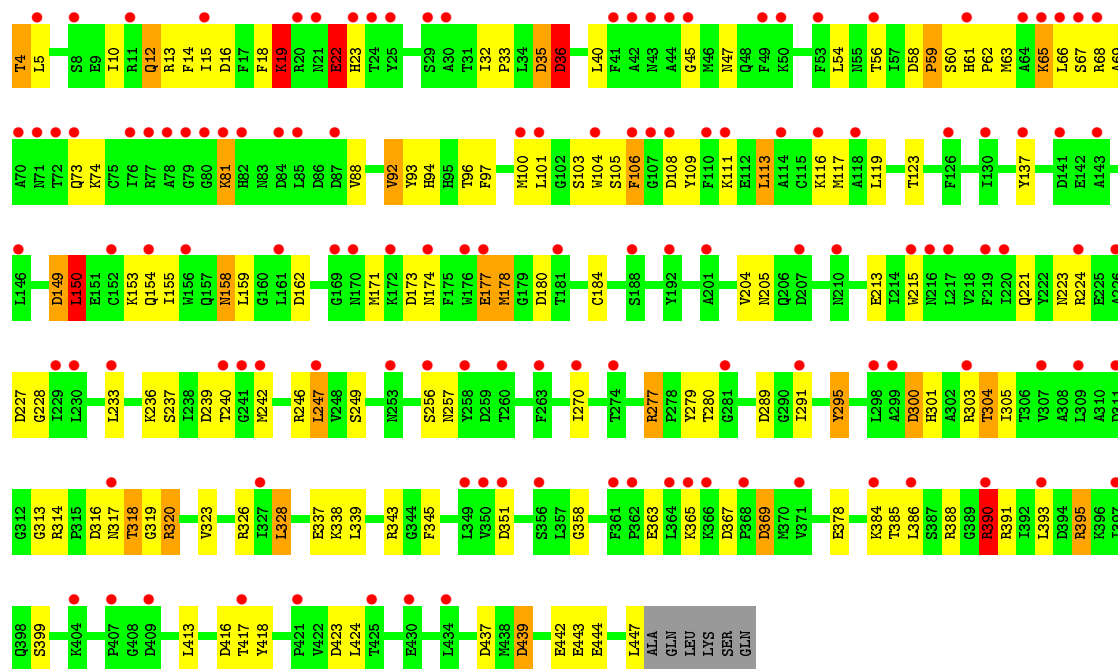
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Alanine-tRNA ligase, cytoplasmic

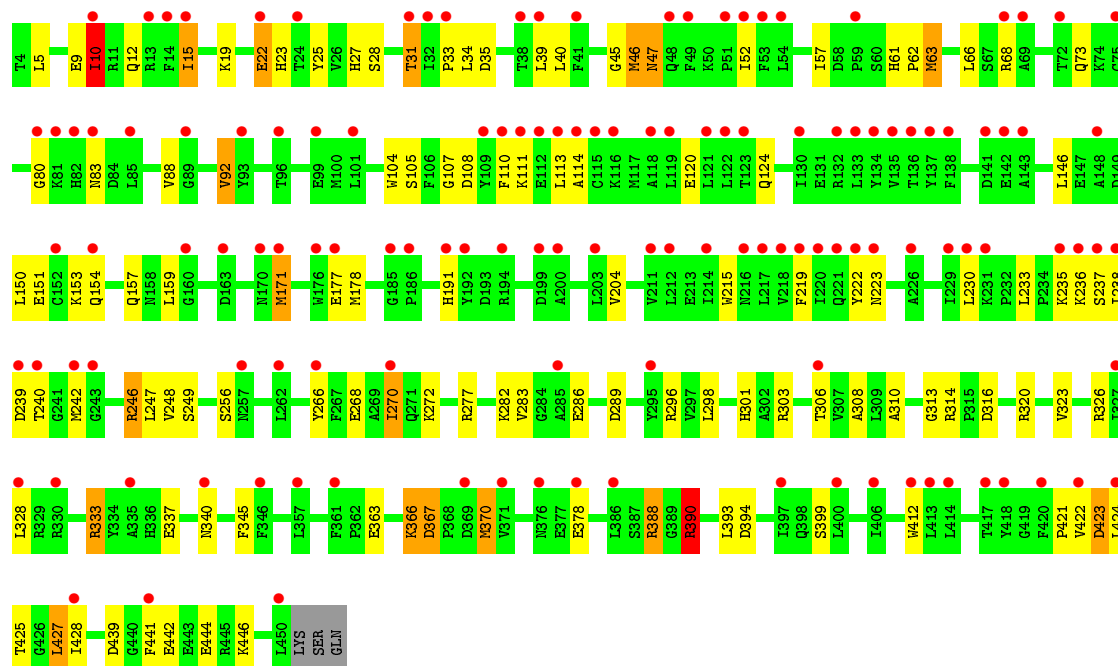
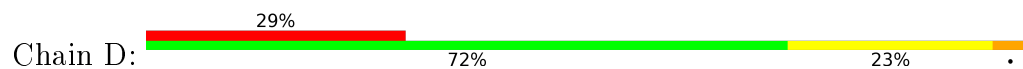


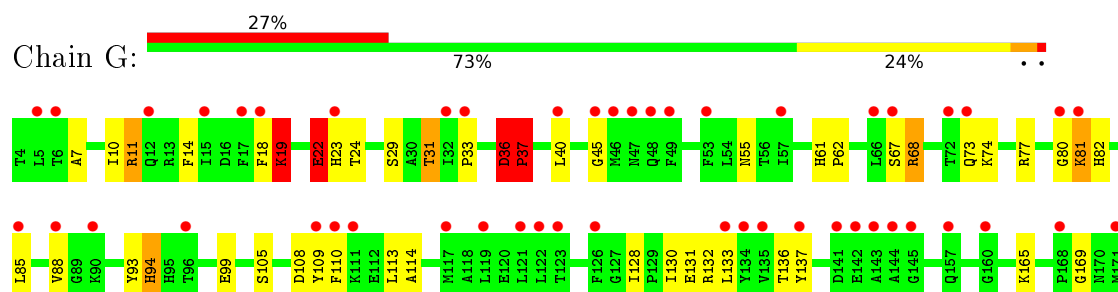
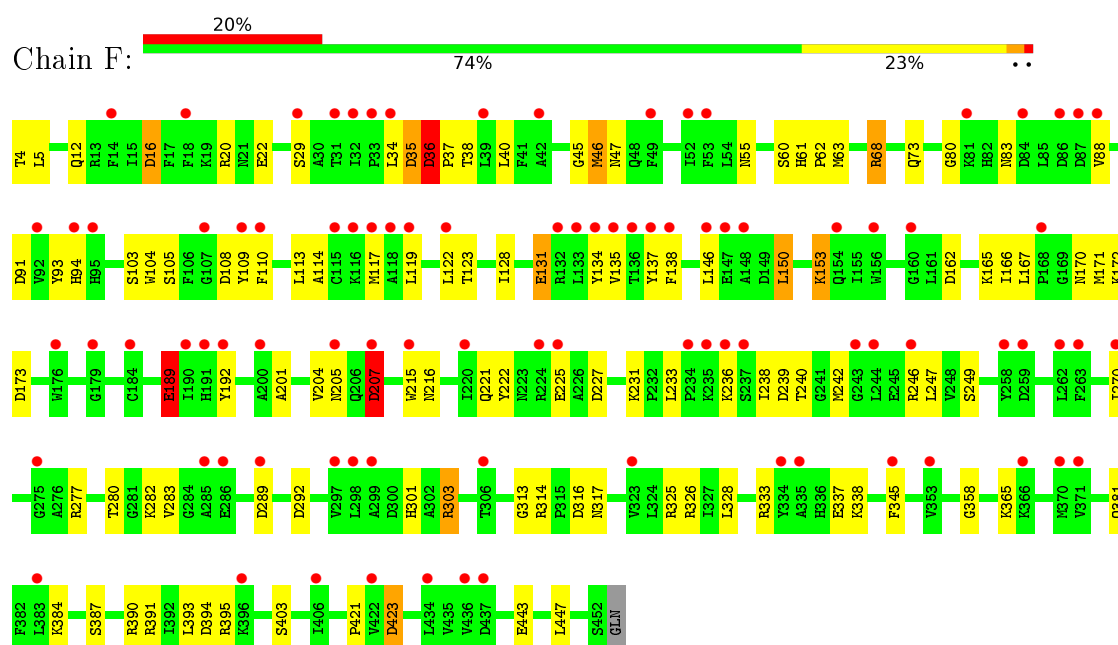
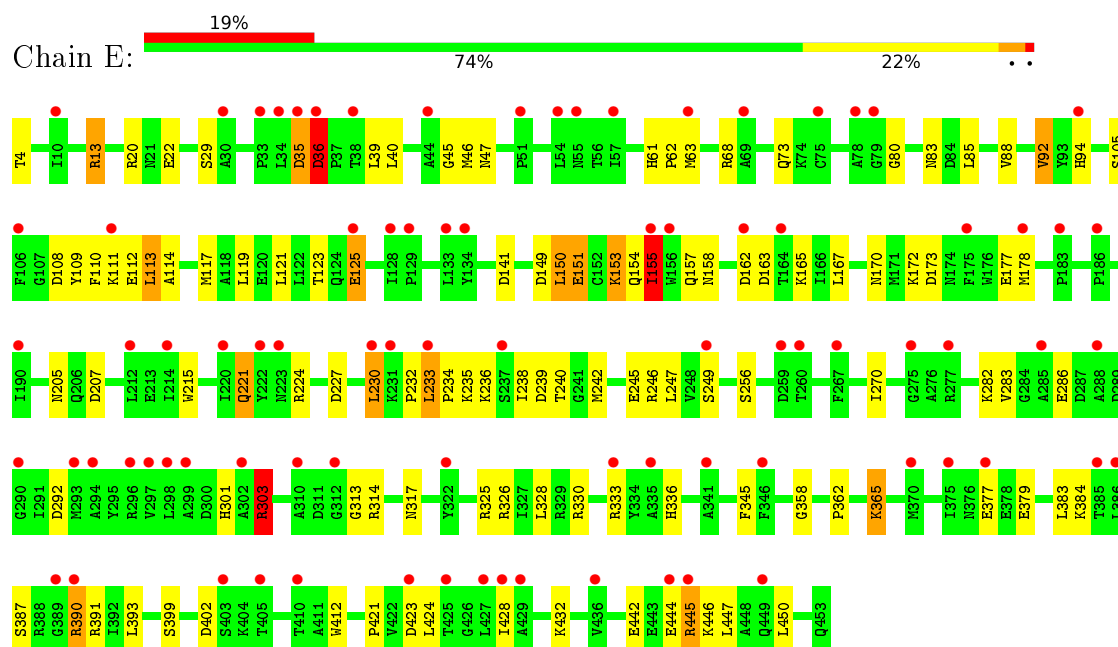


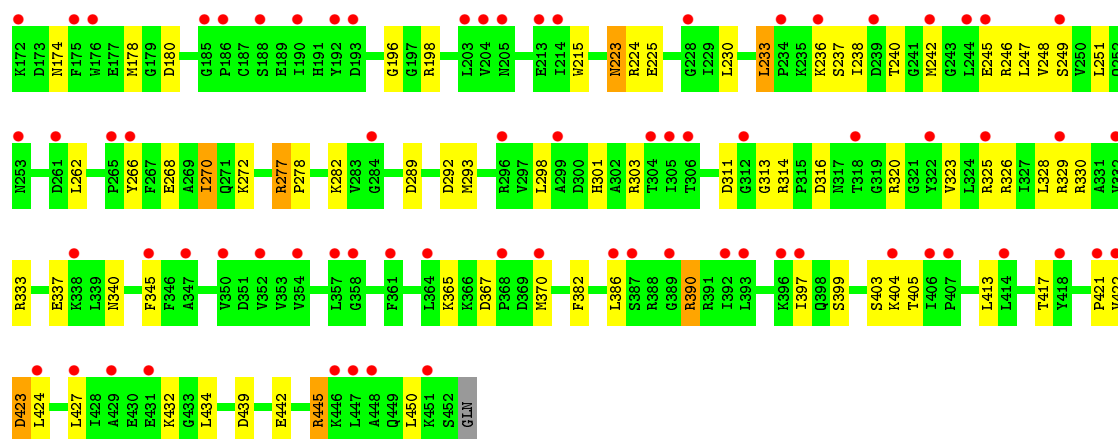
• Molecule 1: Alanine-tRNA ligase, cytoplasmic



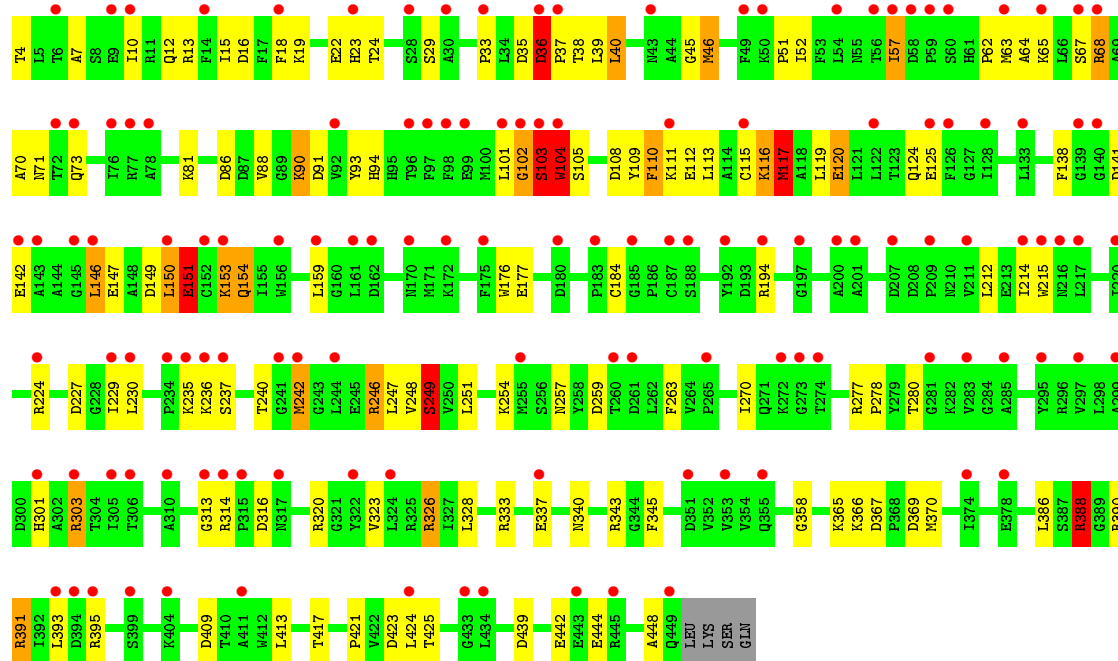
• Molecule 1: Alanine-tRNA ligase, cytoplasmic







• Molecule 1: Alanine-tRNA ligase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.17 Å 98.26 Å 201.38 Å 90.07° 89.95° 90.11°	Depositor
Resolution (Å)	49.13 – 2.68 49.13 – 2.68	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.13-2.68) 99.4 (49.13-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.69 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.254 0.282 , 0.318	Depositor DCC
R_{free} test set	5431 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l 0.079 for -h,k,-l 0.146 for -h,-k,l	Xtriage
Reported twinning fraction	0.441 for H, K, L 0.076 for -H, -K, L 0.275 for H, -K, -L 0.209 for -H, K, -L	Depositor
Outliers	0 of 112184 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	28584	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: A5A

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	0.77	1/3635 (0.0%)	1.01	22/4915 (0.4%)
1	B	0.78	4/3635 (0.1%)	1.01	26/4915 (0.5%)
1	C	0.86	6/3589 (0.2%)	1.16	39/4854 (0.8%)
1	D	0.81	2/3611 (0.1%)	1.11	29/4884 (0.6%)
1	E	0.79	2/3635 (0.1%)	1.04	26/4915 (0.5%)
1	F	0.80	1/3626 (0.0%)	0.99	22/4903 (0.4%)
1	G	0.81	0/3626	1.08	28/4903 (0.6%)
1	H	0.87	5/3603 (0.1%)	1.16	36/4873 (0.7%)
All	All	0.81	21/28960 (0.1%)	1.07	228/39162 (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	B	0	2
1	C	0	2
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	4
All	All	0	12

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	151	GLU	C-O	-7.96	1.08	1.23
1	C	149	ASP	CG-OD2	-7.35	1.08	1.25
1	C	442	GLU	CD-OE1	7.21	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	GLU	CD-OE1	6.73	1.33	1.25
1	B	177	GLU	CD-OE1	-6.72	1.18	1.25
1	C	177	GLU	CG-CD	-6.71	1.41	1.51
1	F	134	TYR	CB-CG	-6.40	1.42	1.51
1	B	189	GLU	CD-OE1	-6.30	1.18	1.25
1	H	102	GLY	N-CA	5.79	1.54	1.46
1	B	256	SER	CA-CB	5.63	1.61	1.52
1	B	213	GLU	CG-CD	5.57	1.60	1.51
1	C	19	LYS	CB-CG	5.50	1.67	1.52
1	C	439	ASP	CB-CG	-5.39	1.40	1.51
1	D	366	LYS	CA-CB	5.34	1.65	1.53
1	H	101	LEU	C-O	-5.33	1.13	1.23
1	H	115	CYS	CB-SG	-5.27	1.73	1.81
1	A	177	GLU	CD-OE1	-5.23	1.19	1.25
1	C	74	LYS	CD-CE	5.16	1.64	1.51
1	E	46	MET	CG-SD	-5.08	1.68	1.81
1	H	249	SER	CA-CB	5.01	1.60	1.52
1	E	125	GLU	CD-OE2	-5.00	1.20	1.25

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ASP	CB-CG-OD1	13.34	130.31	118.30
1	E	402	ASP	CB-CG-OD2	-12.89	106.70	118.30
1	H	303	ARG	NE-CZ-NH1	11.53	126.07	120.30
1	D	367	ASP	CB-CG-OD1	11.23	128.41	118.30
1	D	367	ASP	CB-CG-OD2	-10.24	109.09	118.30
1	A	277	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	E	163	ASP	CB-CG-OD2	9.83	127.15	118.30
1	E	365	LYS	CD-CE-NZ	-9.75	89.27	111.70
1	B	68	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	E	230	LEU	CB-CG-CD1	9.45	127.06	111.00
1	C	300	ASP	CB-CG-OD2	9.23	126.61	118.30
1	A	277	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	C	162	ASP	CB-CG-OD2	9.03	126.43	118.30
1	D	146	LEU	CB-CG-CD1	9.03	126.35	111.00
1	H	102	GLY	N-CA-C	8.94	135.46	113.10
1	F	36	ASP	CB-CG-OD1	8.71	126.14	118.30
1	D	439	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	H	388	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	303	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	B	242	MET	CG-SD-CE	8.35	113.57	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	35	ASP	CB-CG-OD1	-8.35	110.78	118.30
1	H	90	LYS	CB-CG-CD	8.35	133.31	111.60
1	H	103	SER	N-CA-C	8.34	133.53	111.00
1	C	390	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	G	130	ILE	CA-CB-CG2	8.31	127.52	110.90
1	H	242	MET	CG-SD-CE	8.30	113.47	100.20
1	G	325	ARG	CG-CD-NE	8.26	129.15	111.80
1	E	36	ASP	CB-CG-OD1	8.26	125.73	118.30
1	A	326	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	C	295	TYR	CB-CG-CD1	8.23	125.94	121.00
1	H	391	ARG	CA-CB-CG	8.20	131.44	113.40
1	E	303	ARG	CG-CD-NE	-8.16	94.66	111.80
1	G	439	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	G	329	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	E	402	ASP	CB-CG-OD1	8.01	125.50	118.30
1	G	316	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	H	117	MET	CA-CB-CG	7.99	126.88	113.30
1	H	224	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	H	35	ASP	CB-CG-OD2	7.91	125.42	118.30
1	F	35	ASP	CB-CG-OD1	7.87	125.38	118.30
1	B	146	LEU	CB-CG-CD1	7.85	124.34	111.00
1	F	146	LEU	CB-CG-CD1	7.84	124.34	111.00
1	B	35	ASP	CB-CG-OD1	7.84	125.36	118.30
1	H	212	LEU	CA-CB-CG	7.78	133.19	115.30
1	B	36	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	H	91	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	36	ASP	CB-CG-OD2	7.55	125.09	118.30
1	H	388	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	171	MET	CG-SD-CE	7.52	112.23	100.20
1	C	247	LEU	CB-CG-CD2	-7.46	98.31	111.00
1	B	230	LEU	CA-CB-CG	-7.42	98.22	115.30
1	D	390	ARG	CD-NE-CZ	7.30	133.82	123.60
1	F	35	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	C	22	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	E	35	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	C	149	ASP	OD1-CG-OD2	-7.25	109.53	123.30
1	C	277	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	B	40	LEU	CB-CG-CD1	7.20	123.23	111.00
1	H	36	ASP	CB-CG-OD1	7.19	124.78	118.30
1	H	46	MET	CB-CG-SD	7.18	133.93	112.40
1	E	35	ASP	CB-CG-OD1	7.13	124.72	118.30
1	H	343	ARG	NE-CZ-NH1	7.13	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	316	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	G	316	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	221	GLN	N-CA-CB	-7.10	97.82	110.60
1	D	22	GLU	N-CA-C	6.99	129.88	111.00
1	F	16	ASP	CB-CG-OD2	6.97	124.58	118.30
1	C	13	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	G	329	ARG	CD-NE-CZ	6.95	133.33	123.60
1	D	316	ASP	CB-CG-OD1	6.94	124.54	118.30
1	C	395	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	343	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	F	40	LEU	CB-CG-CD1	6.84	122.63	111.00
1	G	445	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	36	ASP	C-N-CD	-6.80	105.64	120.60
1	G	36	ASP	CB-CG-OD1	6.74	124.36	118.30
1	G	233	LEU	CA-CB-CG	6.71	130.73	115.30
1	A	40	LEU	CB-CG-CD2	6.65	122.31	111.00
1	D	108	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	B	48	GLN	CB-CG-CD	6.64	128.87	111.60
1	C	106	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	D	63	MET	CG-SD-CE	6.62	110.80	100.20
1	C	150	LEU	CA-CB-CG	6.62	130.53	115.30
1	A	445	ARG	CG-CD-NE	6.54	125.55	111.80
1	E	121	LEU	CB-CG-CD2	-6.52	99.91	111.00
1	F	68	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	C	338	LYS	CD-CE-NZ	6.49	126.62	111.70
1	B	68	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	C	416	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	120	GLU	OE1-CD-OE2	-6.47	115.54	123.30
1	G	282	LYS	CD-CE-NZ	-6.43	96.91	111.70
1	B	35	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	G	293	MET	CA-CB-CG	6.41	124.19	113.30
1	C	390	ARG	CD-NE-CZ	6.37	132.52	123.60
1	D	316	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	D	388	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	E	13	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	E	163	ASP	OD1-CG-OD2	-6.31	111.31	123.30
1	G	270	ILE	CA-CB-CG1	6.31	122.98	111.00
1	G	88	VAL	N-CA-C	6.30	128.00	111.00
1	C	295	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	B	63	MET	CG-SD-CE	6.17	110.08	100.20
1	F	447	LEU	CA-CB-CG	6.16	129.47	115.30
1	C	439	ASP	CB-CG-OD1	-6.15	112.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	225	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	H	104	TRP	N-CA-C	6.14	127.59	111.00
1	H	68	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	277	ARG	CB-CA-C	6.08	122.57	110.40
1	E	141	ASP	CB-CG-OD2	6.08	123.77	118.30
1	H	40	LEU	CB-CG-CD2	-6.06	100.69	111.00
1	B	162	ASP	CB-CG-OD1	6.05	123.75	118.30
1	E	153	LYS	N-CA-CB	6.05	121.48	110.60
1	H	224	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	E	292	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	20	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	F	131	GLU	CB-CA-C	5.93	122.26	110.40
1	A	434	LEU	CB-CG-CD2	5.90	121.04	111.00
1	A	141	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	40	LEU	CB-CG-CD2	-5.89	100.98	111.00
1	D	246	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	270	ILE	CA-CB-CG1	5.87	122.15	111.00
1	F	63	MET	CA-CB-CG	5.87	123.27	113.30
1	G	223	ASN	N-CA-CB	-5.87	100.04	110.60
1	C	390	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	F	303	ARG	CG-CD-NE	5.83	124.05	111.80
1	B	213	GLU	OE1-CD-OE2	-5.81	116.32	123.30
1	D	370	MET	CB-CG-SD	5.81	129.82	112.40
1	C	108	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	296	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	328	LEU	CA-CB-CG	-5.77	102.02	115.30
1	H	303	ARG	CD-NE-CZ	5.76	131.67	123.60
1	A	154	GLN	CA-CB-CG	5.74	126.03	113.40
1	D	439	ASP	CB-CG-OD1	5.74	123.47	118.30
1	G	68	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	106	PHE	CB-CG-CD2	5.71	124.79	120.80
1	H	57	ILE	CA-CB-CG2	5.70	122.30	110.90
1	A	393	LEU	CB-CG-CD2	5.69	120.67	111.00
1	C	393	LEU	CB-CG-CD2	5.68	120.66	111.00
1	D	10	ILE	CA-CB-CG2	5.68	122.27	110.90
1	C	162	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	D	246	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	G	439	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	171	MET	CA-CB-CG	5.65	122.91	113.30
1	A	326	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	F	134	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	E	167	LEU	CA-CB-CG	5.63	128.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	177	GLU	CG-CD-OE2	5.61	129.52	118.30
1	F	303	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	E	390	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	236	LYS	N-CA-CB	-5.58	100.55	110.60
1	B	236	LYS	CA-CB-CG	5.58	125.67	113.40
1	D	427	LEU	CB-CA-C	-5.58	99.61	110.20
1	B	277	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	H	343	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	F	40	LEU	CB-CG-CD2	-5.57	101.54	111.00
1	B	63	MET	CA-CB-CG	5.56	122.76	113.30
1	C	22	GLU	N-CA-C	5.56	126.00	111.00
1	F	162	ASP	CB-CG-OD1	5.56	123.30	118.30
1	H	103	SER	CB-CA-C	-5.53	99.60	110.10
1	F	393	LEU	CB-CG-CD2	5.52	120.38	111.00
1	A	177	GLU	CG-CD-OE1	-5.51	107.28	118.30
1	B	150	LEU	CB-CG-CD1	5.50	120.36	111.00
1	F	150	LEU	CB-CG-CD1	5.50	120.35	111.00
1	B	120	GLU	CG-CD-OE1	5.50	129.30	118.30
1	C	304	THR	CA-CB-CG2	-5.50	104.70	112.40
1	G	22	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	E	150	LEU	CB-CG-CD1	5.49	120.33	111.00
1	D	124	GLN	N-CA-CB	5.48	120.46	110.60
1	A	316	ASP	CB-CG-OD1	5.46	123.21	118.30
1	H	40	LEU	CB-CG-CD1	5.42	120.21	111.00
1	E	46	MET	CG-SD-CE	5.41	108.86	100.20
1	F	207	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	H	391	ARG	CB-CA-C	-5.40	99.60	110.40
1	A	13	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	388	ARG	N-CA-CB	5.39	120.30	110.60
1	F	153	LYS	CD-CE-NZ	5.39	124.09	111.70
1	F	189	GLU	CA-CB-CG	5.38	125.25	113.40
1	E	113	LEU	CB-CG-CD2	5.37	120.13	111.00
1	C	424	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	E	155	ILE	CG1-CB-CG2	5.34	123.15	111.40
1	B	46	MET	CG-SD-CE	5.33	108.73	100.20
1	H	303	ARG	CG-CD-NE	5.33	123.00	111.80
1	G	390	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	35	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	G	19	LYS	CD-CE-NZ	5.29	123.86	111.70
1	C	320	ARG	CG-CD-NE	-5.26	100.75	111.80
1	H	246	ARG	N-CA-CB	-5.26	101.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	22	GLU	N-CA-C	5.25	125.18	111.00
1	C	247	LEU	CB-CG-CD1	5.25	119.92	111.00
1	B	157	GLN	N-CA-CB	5.23	120.01	110.60
1	E	393	LEU	CB-CG-CD2	5.22	119.88	111.00
1	H	395	ARG	N-CA-CB	5.21	119.97	110.60
1	E	379	GLU	N-CA-CB	5.19	119.95	110.60
1	E	227	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	450	LEU	CB-CG-CD2	5.19	119.82	111.00
1	F	20	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	H	110	PHE	CB-CA-C	5.17	120.75	110.40
1	G	277	ARG	CG-CD-NE	-5.17	100.94	111.80
1	G	293	MET	CB-CA-C	-5.17	100.06	110.40
1	D	333	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	282	LYS	CD-CE-NZ	5.16	123.57	111.70
1	H	391	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	G	37	PRO	N-CA-C	5.15	125.49	112.10
1	E	303	ARG	CB-CA-C	5.15	120.69	110.40
1	C	318	THR	CA-CB-CG2	5.14	119.59	112.40
1	D	303	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	F	36	ASP	OD1-CG-OD2	-5.13	113.55	123.30
1	H	247	LEU	CB-CG-CD1	5.12	119.71	111.00
1	C	395	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	113	LEU	CB-CG-CD2	5.11	119.68	111.00
1	H	68	ARG	N-CA-CB	-5.10	101.42	110.60
1	D	34	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	141	ASP	OD1-CG-OD2	-5.09	113.62	123.30
1	C	213	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	D	159	LEU	CB-CG-CD1	5.08	119.64	111.00
1	E	108	ASP	CB-CG-OD1	5.08	122.88	118.30
1	G	450	LEU	CB-CG-CD2	5.08	119.64	111.00
1	C	65	LYS	CA-CB-CG	5.08	124.57	113.40
1	A	283	VAL	CA-CB-CG2	5.07	118.51	110.90
1	C	439	ASP	N-CA-CB	5.06	119.70	110.60
1	D	35	ASP	CB-CG-OD1	5.05	122.84	118.30
1	G	434	LEU	CB-CG-CD2	5.03	119.55	111.00
1	B	113	LEU	CB-CG-CD2	5.02	119.53	111.00
1	A	240	THR	N-CA-CB	5.01	119.83	110.30
1	H	303	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	G	81	LYS	N-CA-C	5.01	124.52	111.00
1	C	19	LYS	CD-CE-NZ	5.00	123.21	111.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	LYS	Peptide
1	B	277	ARG	Peptide
1	B	36	ASP	Peptide
1	C	22	GLU	Peptide
1	C	36	ASP	Peptide
1	E	36	ASP	Peptide
1	F	36	ASP	Peptide
1	G	36	ASP	Peptide
1	H	117	MET	Peptide
1	H	150	LEU	Peptide
1	H	151	GLU	Peptide
1	H	36	ASP	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	3560	0	3499	56	1
1	B	3560	0	3499	90	0
1	C	3514	0	3449	127	0
1	D	3536	0	3473	79	1
1	E	3560	0	3499	79	2
1	F	3551	0	3491	79	2
1	G	3551	0	3491	86	1
1	H	3528	0	3462	119	1
2	A	28	0	19	1	0
2	B	28	0	19	0	0
2	C	28	0	19	3	0
2	D	28	0	19	1	0
2	E	28	0	19	2	0
2	F	28	0	19	0	0
2	G	28	0	19	0	0
2	H	28	0	19	0	0
All	All	28584	0	28015	692	4

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 12.

All (692) 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:277:ARG:NH2	1:A:289:ASP:OD2	1.76	1.18
1:H:40:LEU:O	1:H:320:ARG:NH1	1.84	1.10
1:H:10:ILE:HD11	1:H:251:LEU:HD12	1.16	1.09
1:F:153:LYS:CE	1:F:166:ILE:HG23	1.86	1.04
1:B:222:TYR:HB3	1:B:230:LEU:HD22	1.39	1.01
1:C:54:LEU:HD22	1:C:223:ASN:HD22	1.27	0.98
1:F:153:LYS:HE2	1:F:166:ILE:HG23	1.46	0.97
1:B:222:TYR:HB3	1:B:230:LEU:CD2	1.95	0.97
1:G:233:LEU:O	1:G:236:LYS:NZ	1.99	0.96
1:E:442:GLU:O	1:E:445:ARG:NH1	2.04	0.91
1:H:10:ILE:HD11	1:H:251:LEU:CD1	2.01	0.91
1:H:52:ILE:O	1:H:235:LYS:NZ	2.06	0.89
1:F:381:GLN:OE1	1:F:384:LYS:NZ	2.05	0.89
1:D:233:LEU:O	1:D:236:LYS:NZ	2.07	0.88
1:G:31:THR:OG1	1:G:311:ASP:OD2	1.92	0.88
1:G:74:LYS:NZ	1:G:311:ASP:OD2	2.08	0.87
1:C:242:MET:HE1	1:C:247:LEU:HD12	1.56	0.85
1:H:70:ALA:HA	1:H:104:TRP:CE3	2.13	0.84
1:F:153:LYS:HE3	1:F:166:ILE:HG23	1.57	0.84
1:C:116:LYS:HA	1:C:159:LEU:HD21	1.60	0.84
1:D:326:ARG:NE	1:D:423:ASP:OD2	2.11	0.84
1:C:18:PHE:O	1:C:23:HIS:N	2.09	0.84
1:G:10:ILE:HD11	1:G:251:LEU:HD12	1.60	0.83
1:H:7:ALA:O	1:H:10:ILE:HG22	1.78	0.83
1:G:7:ALA:O	1:G:10:ILE:HG22	1.79	0.81
1:C:10:ILE:CG2	1:C:247:LEU:HD21	2.09	0.81
1:C:22:GLU:HB3	1:C:23:HIS:ND1	1.95	0.81
1:F:36:ASP:O	1:F:38:THR:N	2.13	0.81
1:E:358:GLY:O	1:E:365:LYS:NZ	2.12	0.81
1:H:40:LEU:HD21	1:H:323:VAL:HG21	1.63	0.81
1:B:282:LYS:HG3	1:B:292:ASP:OD2	1.80	0.81
1:H:141:ASP:H	1:H:146:LEU:HD11	1.46	0.80
1:H:39:LEU:O	1:H:320:ARG:NH2	2.14	0.80
1:F:189:GLU:OE1	1:F:216:ASN:ND2	2.11	0.80
1:H:113:LEU:HA	1:H:116:LYS:HB2	1.62	0.80
1:H:10:ILE:CD1	1:H:251:LEU:HD12	2.06	0.80
1:E:215:TRP:HE1	1:E:240:THR:HG23	1.48	0.79
1:G:105:SER:O	1:G:237:SER:OG	2.00	0.79
1:F:215:TRP:HE1	1:F:240:THR:HG23	1.47	0.79
1:H:409:ASP:OD1	1:H:444:GLU:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:SER:O	1:H:237:SER:OG	2.01	0.78
1:D:105:SER:O	1:D:237:SER:OG	2.01	0.78
1:G:10:ILE:CD1	1:G:251:LEU:HD12	2.14	0.78
1:B:68:ARG:HH11	1:B:109:TYR:HD2	1.30	0.78
1:G:40:LEU:HD21	1:G:323:VAL:HG21	1.66	0.78
1:H:70:ALA:HA	1:H:104:TRP:CZ3	2.18	0.78
1:H:36:ASP:O	1:H:38:THR:N	2.14	0.77
1:G:10:ILE:HG21	1:G:248:VAL:HG22	1.66	0.77
1:C:385:THR:HG21	1:C:418:TYR:O	1.84	0.77
1:C:105:SER:O	1:C:237:SER:OG	2.02	0.77
1:A:277:ARG:NH2	1:A:291:ILE:HD12	2.00	0.76
1:B:131:GLU:O	1:B:165:LYS:NZ	2.17	0.76
1:C:242:MET:CE	1:C:247:LEU:HD12	2.14	0.76
1:B:36:ASP:O	1:B:38:THR:N	2.15	0.76
1:D:40:LEU:HD21	1:D:323:VAL:HG21	1.66	0.76
1:B:68:ARG:HD3	1:B:109:TYR:CE2	2.21	0.76
1:C:279:TYR:HB2	1:C:295:TYR:CD2	2.21	0.76
1:C:40:LEU:HD21	1:C:323:VAL:HG21	1.67	0.76
1:G:326:ARG:NE	1:G:423:ASP:OD2	2.19	0.76
1:E:233:LEU:HG	1:E:235:LYS:O	1.86	0.76
1:E:224:ARG:HH21	1:E:230:LEU:HD11	1.49	0.75
1:C:96:THR:HB	1:C:304:THR:HG21	1.68	0.75
1:C:81:LYS:NZ	1:C:180:ASP:OD1	2.19	0.75
1:D:268:GLU:O	1:D:272:LYS:HG3	1.86	0.75
1:G:114:ALA:HB2	1:G:238:ILE:HD13	1.69	0.74
1:G:268:GLU:O	1:G:272:LYS:HG3	1.87	0.74
1:B:128:ILE:HD11	1:B:133:LEU:HD11	1.70	0.74
1:B:215:TRP:HE1	1:B:240:THR:HG23	1.51	0.74
1:C:277:ARG:NH1	1:C:289:ASP:OD2	2.21	0.74
1:D:215:TRP:HE1	1:D:240:THR:HG23	1.51	0.74
1:G:215:TRP:HE1	1:G:240:THR:HG23	1.52	0.74
1:H:102:GLY:O	1:H:104:TRP:CD2	2.41	0.74
1:H:215:TRP:HE1	1:H:240:THR:HG23	1.53	0.74
1:C:4:THR:HG22	1:C:5:LEU:HD12	1.68	0.73
1:B:114:ALA:HB2	1:B:238:ILE:HD13	1.69	0.73
1:C:337:GLU:OE1	1:C:390:ARG:NH1	2.20	0.73
1:D:114:ALA:HB2	1:D:238:ILE:HD13	1.70	0.73
1:H:10:ILE:HG21	1:H:248:VAL:HG22	1.70	0.73
1:C:246:ARG:HA	1:C:257:ASN:OD1	1.88	0.73
1:F:280:THR:HG23	1:F:282:LYS:HG3	1.71	0.73
1:E:61:HIS:HA	1:G:340:ASN:HD21	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:ARG:NH1	1:F:289:ASP:OD2	2.21	0.73
1:H:151:GLU:HA	1:H:154:GLN:H	1.54	0.72
1:E:13:ARG:NH1	1:E:20:ARG:HH12	1.87	0.72
1:G:223:ASN:HD22	1:G:233:LEU:HD12	1.54	0.72
1:G:22:GLU:O	1:G:68:ARG:NH1	2.23	0.71
1:A:61:HIS:HA	1:D:340:ASN:HD21	1.54	0.71
1:E:215:TRP:HE1	1:E:240:THR:CG2	2.03	0.71
1:E:282:LYS:HD2	1:E:286:GLU:O	1.91	0.71
1:B:122:LEU:HB3	1:B:128:ILE:HG12	1.71	0.71
1:C:215:TRP:HE1	1:C:240:THR:HG23	1.54	0.71
1:D:110:PHE:HE1	1:D:219:PHE:HB3	1.56	0.71
1:F:114:ALA:HB2	1:F:238:ILE:HD13	1.70	0.71
1:D:110:PHE:CE1	1:D:219:PHE:HB3	2.25	0.71
1:F:215:TRP:HE1	1:F:240:THR:CG2	2.04	0.71
1:F:204:VAL:O	1:F:205:ASN:HB3	1.90	0.71
1:E:114:ALA:HB2	1:E:238:ILE:HD13	1.70	0.70
1:E:150:LEU:HA	1:E:153:LYS:HG3	1.72	0.70
2:C:500:A5A:H5'1	2:C:500:A5A:H8	1.72	0.70
1:A:114:ALA:HB2	1:A:238:ILE:HD13	1.73	0.70
1:H:67:SER:HB2	1:H:108:ASP:HB2	1.73	0.70
1:H:116:LYS:O	1:H:117:MET:HG2	1.92	0.70
1:B:215:TRP:HE1	1:B:240:THR:CG2	2.05	0.70
1:C:177:GLU:HG3	1:C:184:CYS:HB3	1.74	0.70
1:G:61:HIS:CD2	1:G:62:PRO:HD2	2.27	0.69
1:F:61:HIS:HA	1:H:340:ASN:HD21	1.57	0.69
1:C:391:ARG:HE	1:C:395:ARG:HD2	1.57	0.69
1:H:19:LYS:HA	1:H:23:HIS:H	1.58	0.69
1:D:63:MET:HA	1:D:66:LEU:HD13	1.74	0.69
1:A:337:GLU:OE1	1:A:390:ARG:NH1	2.26	0.69
1:C:137:TYR:C	1:C:174:ASN:HD22	1.96	0.69
1:H:117:MET:HB3	1:H:120:GLU:HB2	1.75	0.69
1:C:23:HIS:HA	1:C:68:ARG:HG3	1.75	0.68
1:F:34:LEU:HB3	1:H:277:ARG:NH2	2.09	0.68
1:G:424:LEU:HD12	1:G:427:LEU:HD11	1.75	0.68
1:G:22:GLU:HB3	1:G:68:ARG:CZ	2.23	0.68
1:A:280:THR:HG23	1:A:282:LYS:HG3	1.76	0.68
1:C:279:TYR:HB2	1:C:295:TYR:CE2	2.28	0.68
1:C:33:PRO:HB2	1:C:36:ASP:OD2	1.93	0.68
1:C:351:ASP:OD2	1:E:232:PRO:HD3	1.95	0.67
1:B:85:LEU:O	1:B:88:VAL:HG22	1.93	0.67
1:H:19:LYS:HB2	1:H:23:HIS:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:TRP:HE1	1:H:240:THR:CG2	2.06	0.67
1:E:13:ARG:HD2	1:E:125:GLU:OE1	1.94	0.67
1:F:35:ASP:HB2	1:H:277:ARG:HB2	1.77	0.67
1:C:385:THR:HG21	1:C:418:TYR:CA	2.24	0.67
1:E:221:GLN:HB2	1:E:236:LYS:HD2	1.77	0.67
1:B:68:ARG:HD3	1:B:109:TYR:HE2	1.59	0.67
1:C:215:TRP:HE1	1:C:240:THR:CG2	2.08	0.66
1:D:215:TRP:HE1	1:D:240:THR:CG2	2.08	0.66
1:G:85:LEU:HD11	1:G:330:ARG:NH1	2.11	0.66
1:G:85:LEU:HD11	1:G:330:ARG:HH12	1.60	0.66
1:A:282:LYS:HD2	1:A:286:GLU:O	1.96	0.66
1:C:10:ILE:HG21	1:C:247:LEU:HD21	1.76	0.66
1:D:266:TYR:O	1:D:270:ILE:HG12	1.96	0.66
1:G:215:TRP:HE1	1:G:240:THR:CG2	2.09	0.66
1:H:40:LEU:O	1:H:320:ARG:CZ	2.44	0.65
1:C:113:LEU:O	1:C:117:MET:HG2	1.96	0.65
1:C:19:LYS:HG2	1:C:23:HIS:O	1.97	0.65
1:C:100:MET:HE2	2:C:500:A5A:H5'2	1.76	0.65
1:G:68:ARG:HB2	1:G:68:ARG:NH1	2.12	0.65
1:E:221:GLN:O	1:E:221:GLN:HG3	1.96	0.65
1:A:40:LEU:O	1:A:320:ARG:HD3	1.95	0.64
1:H:141:ASP:H	1:H:146:LEU:CD1	2.09	0.64
1:G:68:ARG:HH11	1:G:68:ARG:HB2	1.62	0.64
1:C:54:LEU:HD22	1:C:223:ASN:ND2	2.05	0.64
1:C:119:LEU:O	1:C:123:THR:OG1	2.16	0.64
1:A:119:LEU:O	1:A:123:THR:OG1	2.14	0.64
1:A:289:ASP:OD1	1:A:289:ASP:N	2.30	0.64
1:B:119:LEU:O	1:B:123:THR:OG1	2.15	0.64
1:D:235:LYS:HD2	1:D:236:LYS:H	1.62	0.64
1:E:215:TRP:NE1	1:E:240:THR:HG23	2.13	0.64
1:E:119:LEU:O	1:E:123:THR:OG1	2.15	0.63
1:F:221:GLN:HG2	1:F:236:LYS:HD3	1.79	0.63
1:E:442:GLU:OE2	1:E:445:ARG:HD3	1.98	0.63
1:H:117:MET:HA	1:H:119:LEU:H	1.64	0.63
1:C:351:ASP:OD2	1:E:232:PRO:CD	2.47	0.63
1:D:19:LYS:HB2	1:D:23:HIS:O	1.99	0.63
1:G:330:ARG:HH21	1:G:423:ASP:CB	2.11	0.63
1:F:119:LEU:O	1:F:123:THR:OG1	2.16	0.63
1:H:141:ASP:N	1:H:146:LEU:HD11	2.14	0.63
1:F:215:TRP:NE1	1:F:240:THR:HG23	2.14	0.62
1:H:120:GLU:HG2	1:H:124:GLN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LYS:HG2	1:C:23:HIS:C	2.18	0.62
1:A:277:ARG:CZ	1:A:291:ILE:HD12	2.29	0.62
1:E:412:TRP:CD2	1:E:444:GLU:OE1	2.52	0.62
1:H:388:ARG:O	1:H:391:ARG:HB2	1.98	0.62
1:G:403:SER:O	1:G:404:LYS:HD3	1.98	0.62
1:B:326:ARG:HD3	1:B:423:ASP:OD2	1.99	0.62
1:C:177:GLU:HG3	1:C:184:CYS:CB	2.30	0.62
1:C:23:HIS:HD2	1:C:69:ALA:O	1.82	0.61
1:B:274:THR:O	1:B:276:ALA:N	2.33	0.61
1:F:326:ARG:HG2	1:F:421:PRO:HB3	1.80	0.61
1:C:63:MET:HG3	1:C:66:LEU:HD13	1.82	0.61
1:E:173:ASP:CG	1:E:205:ASN:HD21	2.04	0.61
1:B:122:LEU:O	1:B:128:ILE:HG13	2.00	0.61
1:H:23:HIS:CD2	1:H:68:ARG:HG3	2.36	0.61
1:E:326:ARG:HG2	1:E:421:PRO:HB3	1.81	0.61
1:G:133:LEU:O	1:G:165:LYS:NZ	2.20	0.61
1:A:221:GLN:HG3	1:A:236:LYS:HD2	1.83	0.61
1:B:222:TYR:HB3	1:B:230:LEU:HD21	1.81	0.60
1:C:173:ASP:CG	1:C:205:ASN:HD21	2.05	0.60
1:C:277:ARG:HH21	1:C:280:THR:HG22	1.65	0.60
1:C:385:THR:O	1:C:385:THR:HG22	1.99	0.60
1:D:444:GLU:O	1:D:444:GLU:HG3	2.01	0.60
1:H:111:LYS:NZ	1:H:149:ASP:OD1	2.34	0.60
1:A:277:ARG:HH22	1:A:289:ASP:CG	2.05	0.60
1:F:93:TYR:OH	1:F:207:ASP:OD1	2.19	0.60
1:G:266:TYR:O	1:G:270:ILE:HG12	1.99	0.60
1:E:173:ASP:OD2	1:E:205:ASN:ND2	2.34	0.60
1:F:12:GLN:HG3	1:F:16:ASP:OD2	2.02	0.60
1:E:336:HIS:CD2	1:E:383:LEU:HD21	2.37	0.60
1:C:111:LYS:NZ	1:C:149:ASP:OD1	2.35	0.60
1:C:224:ARG:HE	1:C:228:GLY:HA2	1.65	0.60
1:B:215:TRP:NE1	1:B:240:THR:HG23	2.15	0.60
1:D:47:ASN:H	1:D:47:ASN:HD22	1.48	0.60
1:C:277:ARG:HH21	1:C:280:THR:CG2	2.15	0.59
1:B:68:ARG:NH1	1:B:108:ASP:OD1	2.35	0.59
1:C:385:THR:HG21	1:C:418:TYR:C	2.22	0.59
1:C:385:THR:HG21	1:C:418:TYR:HA	1.83	0.59
1:A:326:ARG:NE	1:A:423:ASP:OD2	2.35	0.59
1:H:102:GLY:O	1:H:104:TRP:CE3	2.55	0.59
1:H:19:LYS:HA	1:H:23:HIS:N	2.17	0.59
1:H:227:ASP:OD2	1:H:229:ILE:HD12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:OD1	1:A:325:ARG:NH2	2.35	0.59
1:G:136:THR:HB	1:G:174:ASN:HD21	1.68	0.59
1:B:36:ASP:OD2	1:B:39:LEU:HB2	2.01	0.59
1:A:61:HIS:HA	1:D:340:ASN:ND2	2.17	0.59
1:H:326:ARG:HG2	1:H:421:PRO:HB3	1.85	0.58
1:C:155:ILE:O	1:C:158:ASN:HB3	2.03	0.58
1:C:15:ILE:HG13	1:C:16:ASP:N	2.17	0.58
1:D:390:ARG:NH1	1:D:394:ASP:OD2	2.36	0.58
1:G:277:ARG:NH1	1:G:289:ASP:OD2	2.36	0.58
1:B:222:TYR:CB	1:B:230:LEU:HD22	2.25	0.58
1:B:29:SER:H	1:B:48:GLN:HE21	1.50	0.58
1:H:22:GLU:HB2	1:H:68:ARG:HH21	1.68	0.58
1:F:153:LYS:HE3	1:F:166:ILE:CG2	2.29	0.58
1:C:391:ARG:NE	1:C:395:ARG:HD2	2.19	0.58
1:D:424:LEU:O	1:D:427:LEU:HB2	2.04	0.58
1:E:233:LEU:HD12	1:E:234:PRO:CD	2.34	0.58
1:B:116:LYS:HA	1:B:159:LEU:HD21	1.84	0.58
1:D:33:PRO:HD2	1:D:320:ARG:NH1	2.20	0.57
1:E:239:ASP:OD2	2:E:500:A5A:N	2.36	0.57
1:B:128:ILE:HD12	1:B:128:ILE:O	2.04	0.57
1:C:173:ASP:OD2	1:C:205:ASN:ND2	2.31	0.57
1:H:62:PRO:O	1:H:65:LYS:HB2	2.04	0.57
1:C:32:ILE:HG23	1:C:320:ARG:HH11	1.69	0.57
1:G:270:ILE:HD12	1:G:298:LEU:HD23	1.85	0.57
1:H:102:GLY:HA3	1:H:240:THR:O	2.05	0.57
1:A:93:TYR:HA	1:A:257:ASN:ND2	2.20	0.57
1:E:162:ASP:H	1:E:165:LYS:HE2	1.69	0.57
1:C:323:VAL:HG22	1:C:326:ARG:HH21	1.69	0.57
1:H:117:MET:SD	1:H:120:GLU:HB2	2.44	0.57
1:D:215:TRP:NE1	1:D:240:THR:HG23	2.20	0.57
1:C:215:TRP:NE1	1:C:240:THR:HG23	2.20	0.56
1:D:110:PHE:HD2	1:D:111:LYS:CG	2.18	0.56
1:F:326:ARG:NE	1:F:423:ASP:OD2	2.38	0.56
1:A:333:ARG:HD3	1:A:424:LEU:HD11	1.86	0.56
1:A:326:ARG:HG2	1:A:421:PRO:HB3	1.87	0.56
1:C:154:GLN:O	1:C:158:ASN:HB2	2.04	0.56
1:E:362:PRO:HA	1:E:365:LYS:NZ	2.21	0.56
1:E:61:HIS:HA	1:G:340:ASN:ND2	2.18	0.56
1:G:424:LEU:HA	1:G:427:LEU:HG	1.88	0.56
1:A:173:ASP:CG	1:A:205:ASN:HD21	2.08	0.56
1:D:22:GLU:HB2	1:D:68:ARG:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:PHE:CE2	1:H:146:LEU:HD22	2.41	0.56
1:H:13:ARG:NH2	1:H:125:GLU:OE1	2.39	0.56
1:F:153:LYS:HE3	1:F:166:ILE:HG12	1.88	0.56
1:G:333:ARG:HD3	1:G:424:LEU:HD11	1.86	0.56
1:H:18:PHE:CE1	1:H:103:SER:HB3	2.41	0.56
1:H:33:PRO:HG2	1:H:320:ARG:HH22	1.70	0.56
1:H:270:ILE:HA	1:H:345:PHE:HZ	1.70	0.56
1:H:112:GLU:O	1:H:116:LYS:N	2.39	0.55
1:B:28:SER:HB3	1:B:73:GLN:HA	1.89	0.55
1:E:246:ARG:NH1	2:E:500:A5A:O2'	2.40	0.55
1:B:221:GLN:HG2	1:B:236:LYS:HE3	1.86	0.55
1:B:280:THR:OG1	1:B:282:LYS:HE3	2.07	0.55
1:H:215:TRP:NE1	1:H:240:THR:HG23	2.19	0.55
1:D:239:ASP:OD2	2:D:500:A5A:N	2.39	0.55
1:G:19:LYS:HB2	1:G:23:HIS:O	2.05	0.55
1:E:317:ASN:OD1	1:E:325:ARG:NH2	2.40	0.55
1:G:215:TRP:NE1	1:G:240:THR:HG23	2.21	0.55
1:F:122:LEU:C	1:F:128:ILE:HG22	2.26	0.55
1:F:128:ILE:HD11	1:F:192:TYR:CE2	2.42	0.55
1:H:313:GLY:O	1:H:314:ARG:NH1	2.37	0.55
1:A:451:LYS:HA	1:A:453:GLN:H	1.71	0.54
1:B:68:ARG:HD3	1:B:109:TYR:CD2	2.42	0.54
1:H:117:MET:HB3	1:H:120:GLU:H	1.72	0.54
1:B:128:ILE:CD1	1:B:133:LEU:HD11	2.35	0.54
1:G:10:ILE:HD11	1:G:247:LEU:HG	1.88	0.54
1:D:333:ARG:NH1	1:D:337:GLU:OE1	2.40	0.54
1:D:46:MET:HG3	1:D:47:ASN:N	2.23	0.54
1:D:33:PRO:HG2	1:D:320:ARG:HH12	1.73	0.54
1:F:46:MET:HG3	1:F:47:ASN:N	2.23	0.54
1:H:333:ARG:HD3	1:H:424:LEU:HD11	1.89	0.54
1:B:358:GLY:HA3	1:B:365:LYS:HE3	1.90	0.54
1:D:111:LYS:HE3	1:D:151:GLU:OE2	2.08	0.54
1:F:358:GLY:HA3	1:F:365:LYS:HE3	1.90	0.54
1:C:10:ILE:HG21	1:C:247:LEU:CD2	2.37	0.54
1:D:367:ASP:OD2	1:D:370:MET:HB2	2.08	0.54
1:B:56:THR:HA	1:E:154:GLN:NE2	2.23	0.54
1:H:19:LYS:HD3	1:H:22:GLU:HA	1.89	0.54
1:H:71:ASN:OD1	1:H:104:TRP:CH2	2.61	0.54
1:E:301:HIS:HE1	1:E:330:ARG:HE	1.54	0.53
1:G:22:GLU:HB3	1:G:68:ARG:NH1	2.24	0.53
1:H:33:PRO:HD2	1:H:320:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LYS:O	1:D:157:GLN:HG3	2.08	0.53
1:D:277:ARG:NH1	1:D:289:ASP:OD2	2.42	0.53
1:H:116:LYS:O	1:H:159:LEU:HD21	2.08	0.53
1:C:62:PRO:O	1:C:65:LYS:HB3	2.09	0.53
1:H:409:ASP:OD1	1:H:444:GLU:CG	2.54	0.53
1:D:328:LEU:CD2	1:D:378:GLU:HB3	2.39	0.53
1:B:55:ASN:ND2	1:E:158:ASN:OD1	2.41	0.53
1:F:173:ASP:CG	1:F:205:ASN:HD21	2.10	0.53
1:D:110:PHE:HD2	1:D:111:LYS:HG2	1.74	0.53
1:C:150:LEU:O	1:C:153:LYS:HB3	2.09	0.53
1:B:223:ASN:O	1:B:230:LEU:HD23	2.08	0.53
1:C:301:HIS:HA	1:C:304:THR:OG1	2.09	0.53
1:E:242:MET:HE1	1:E:247:LEU:HD13	1.91	0.53
1:H:86:ASP:O	1:H:90:LYS:HD3	2.08	0.53
1:F:172:LYS:HG3	1:F:173:ASP:N	2.23	0.53
1:F:22:GLU:OE1	1:F:68:ARG:NH1	2.42	0.53
1:F:242:MET:HE1	1:F:247:LEU:HD13	1.91	0.52
1:A:328:LEU:CD2	1:A:378:GLU:HB3	2.39	0.52
1:E:94:HIS:HD2	1:E:246:ARG:NH2	2.07	0.52
1:F:333:ARG:NH1	1:F:337:GLU:OE1	2.42	0.52
1:G:33:PRO:HG2	1:G:320:ARG:NH2	2.24	0.52
1:E:387:SER:OG	1:E:391:ARG:NH2	2.42	0.52
1:F:105:SER:HB2	1:F:109:TYR:CE2	2.45	0.52
1:F:61:HIS:CA	1:H:340:ASN:HD21	2.23	0.52
1:B:282:LYS:CG	1:B:292:ASP:OD2	2.55	0.52
1:D:12:GLN:O	1:D:15:ILE:HG23	2.09	0.52
1:E:444:GLU:OE1	1:E:444:GLU:C	2.48	0.52
1:A:173:ASP:OD2	1:A:205:ASN:ND2	2.38	0.52
1:C:19:LYS:CG	1:C:23:HIS:O	2.57	0.52
1:D:310:ALA:O	1:D:366:LYS:NZ	2.25	0.52
1:G:81:LYS:NZ	1:G:180:ASP:OD1	2.42	0.52
1:H:57:ILE:HD13	1:H:64:ALA:HB2	1.92	0.52
1:B:22:GLU:CG	1:B:68:ARG:HE	2.22	0.52
1:C:93:TYR:HA	1:C:257:ASN:ND2	2.25	0.52
1:D:222:TYR:CE1	1:D:230:LEU:HD13	2.45	0.52
1:G:242:MET:HE1	1:G:247:LEU:HD13	1.92	0.52
1:A:313:GLY:O	1:A:314:ARG:NH1	2.42	0.52
1:B:336:HIS:CD2	1:B:383:LEU:HD21	2.44	0.52
1:D:242:MET:HE1	1:D:247:LEU:HD13	1.92	0.52
1:G:246:ARG:O	1:G:249:SER:OG	2.18	0.52
1:C:385:THR:HG23	1:C:418:TYR:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ARG:O	1:D:249:SER:OG	2.18	0.52
1:F:131:GLU:HB3	1:F:165:LYS:CE	2.40	0.52
1:H:19:LYS:HE2	1:H:24:THR:HA	1.91	0.52
1:B:128:ILE:HD11	1:B:133:LEU:CD1	2.40	0.51
1:D:47:ASN:HD22	1:D:47:ASN:N	2.07	0.51
1:A:387:SER:OG	1:A:391:ARG:NH2	2.43	0.51
1:C:313:GLY:O	1:C:314:ARG:NH1	2.41	0.51
1:D:39:LEU:HD21	1:D:47:ASN:OD1	2.11	0.51
1:H:12:GLN:OE1	1:H:15:ILE:HD11	2.10	0.51
1:E:61:HIS:CA	1:G:340:ASN:HD21	2.22	0.51
1:B:122:LEU:C	1:B:128:ILE:HG13	2.31	0.51
1:H:117:MET:HB3	1:H:120:GLU:CB	2.38	0.51
1:F:61:HIS:HA	1:H:340:ASN:ND2	2.24	0.51
1:H:358:GLY:HA3	1:H:365:LYS:HE3	1.93	0.51
1:F:280:THR:HG21	1:F:282:LYS:HE3	1.91	0.51
1:G:45:GLY:HA2	1:G:73:GLN:HG2	1.92	0.51
1:C:413:LEU:O	1:C:417:THR:OG1	2.28	0.51
1:A:381:GLN:OE1	1:A:384:LYS:NZ	2.38	0.51
1:C:22:GLU:C	1:C:68:ARG:HD2	2.31	0.51
1:C:100:MET:CE	2:C:500:A5A:H5'2	2.40	0.51
1:G:236:LYS:N	1:G:236:LYS:HD3	2.26	0.50
1:B:313:GLY:O	1:B:314:ARG:NH1	2.43	0.50
1:D:270:ILE:HD12	1:D:298:LEU:HD23	1.92	0.50
1:F:4:THR:OG1	1:F:5:LEU:N	2.42	0.50
1:G:85:LEU:CD1	1:G:330:ARG:HH12	2.23	0.50
1:D:236:LYS:N	1:D:236:LYS:HD3	2.25	0.50
1:F:280:THR:CG2	1:F:282:LYS:HE3	2.41	0.50
1:G:11:ARG:NH1	1:G:99:GLU:OE2	2.45	0.50
1:E:446:LYS:HZ2	1:E:450:LEU:HD11	1.76	0.50
1:G:132:ARG:HH21	1:G:196:GLY:HA3	1.77	0.50
1:E:412:TRP:CG	1:E:444:GLU:OE1	2.64	0.50
1:F:313:GLY:O	1:F:314:ARG:NH1	2.43	0.50
1:H:413:LEU:O	1:H:417:THR:OG1	2.29	0.50
1:C:12:GLN:O	1:C:15:ILE:HG13	2.11	0.50
1:D:222:TYR:CD1	1:D:230:LEU:HD13	2.46	0.50
1:D:45:GLY:HA2	1:D:73:GLN:HG2	1.94	0.50
1:A:52:ILE:HD11	1:A:63:MET:HG2	1.93	0.50
1:E:22:GLU:HB2	1:E:68:ARG:HH11	1.75	0.50
1:H:33:PRO:HD2	1:H:320:ARG:CZ	2.41	0.50
1:G:413:LEU:O	1:G:417:THR:OG1	2.30	0.50
1:C:47:ASN:OD1	1:C:178:MET:SD	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:TRP:CD1	1:D:444:GLU:HG2	2.46	0.49
1:F:317:ASN:OD1	1:F:325:ARG:NH2	2.45	0.49
1:C:10:ILE:HG22	1:C:247:LEU:HD21	1.94	0.49
1:D:282:LYS:HD3	1:D:286:GLU:HB3	1.94	0.49
1:H:33:PRO:CG	1:H:320:ARG:HH22	2.25	0.49
1:H:51:PRO:HB2	1:H:57:ILE:CG2	2.42	0.49
1:A:391:ARG:O	1:A:395:ARG:HG2	2.11	0.49
1:C:385:THR:HG23	1:C:418:TYR:CD2	2.46	0.49
1:A:110:PHE:C	1:A:238:ILE:HD11	2.33	0.49
1:A:46:MET:HG3	1:A:47:ASN:N	2.26	0.49
1:C:358:GLY:HA3	1:C:365:LYS:HE3	1.93	0.49
1:A:170:ASN:ND2	1:A:172:LYS:HE3	2.28	0.49
1:B:154:GLN:HA	1:B:157:GLN:HG2	1.94	0.49
1:E:245:GLU:OE2	1:E:303:ARG:NH2	2.43	0.49
1:G:367:ASP:HB2	1:G:370:MET:HB3	1.93	0.49
1:H:337:GLU:HG2	1:H:390:ARG:HH11	1.77	0.49
1:C:23:HIS:NE2	1:C:109:TYR:OH	2.46	0.49
1:D:57:ILE:HD11	1:D:61:HIS:HD2	1.78	0.49
1:G:128:ILE:HA	1:G:128:ILE:HD13	1.66	0.49
1:E:233:LEU:HD12	1:E:234:PRO:HD2	1.93	0.49
1:F:387:SER:OG	1:F:391:ARG:NH2	2.46	0.49
1:A:214:ILE:O	1:A:242:MET:HG3	2.13	0.48
1:H:153:LYS:HD2	1:H:153:LYS:C	2.33	0.48
1:A:61:HIS:ND1	1:A:62:PRO:HD2	2.28	0.48
1:D:333:ARG:NH1	1:D:428:ILE:HG12	2.28	0.48
1:E:153:LYS:O	1:E:157:GLN:HG3	2.13	0.48
1:E:270:ILE:HA	1:E:345:PHE:HZ	1.76	0.48
1:F:270:ILE:HA	1:F:345:PHE:HZ	1.76	0.48
1:B:104:TRP:CD1	1:B:239:ASP:HA	2.47	0.48
1:A:61:HIS:CA	1:D:340:ASN:HD21	2.23	0.48
1:H:102:GLY:O	1:H:104:TRP:CE2	2.66	0.48
1:B:387:SER:OG	1:B:391:ARG:NH2	2.46	0.48
1:C:277:ARG:NH1	1:C:291:ILE:HB	2.28	0.48
1:C:18:PHE:O	1:C:22:GLU:HB2	2.13	0.48
1:F:91:ASP:OD2	1:F:94:HIS:ND1	2.38	0.48
1:G:277:ARG:NH2	1:G:292:ASP:OD1	2.45	0.48
1:A:451:LYS:HD3	1:A:453:GLN:O	2.14	0.48
1:B:390:ARG:NH1	1:B:394:ASP:OD1	2.36	0.48
1:F:170:ASN:OD1	1:F:171:MET:N	2.45	0.48
1:F:289:ASP:O	1:F:338:LYS:NZ	2.27	0.48
1:H:393:LEU:HD11	1:H:425:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:LEU:CG	1:G:330:ARG:HH12	2.27	0.48
1:H:117:MET:C	1:H:119:LEU:H	2.16	0.48
1:F:93:TYR:CE1	1:F:94:HIS:CE1	3.02	0.48
1:B:128:ILE:HD13	1:B:133:LEU:HG	1.96	0.48
1:C:316:ASP:OD1	1:C:317:ASN:N	2.46	0.48
1:D:27:HIS:CD2	1:D:28:SER:H	2.32	0.48
1:A:277:ARG:HH22	1:A:289:ASP:CB	2.27	0.48
1:B:46:MET:HG3	1:B:47:ASN:N	2.28	0.48
1:C:23:HIS:CD2	1:C:69:ALA:O	2.65	0.48
1:B:270:ILE:HA	1:B:345:PHE:HZ	1.79	0.47
1:C:45:GLY:HA2	1:C:73:GLN:HG2	1.96	0.47
1:D:363:GLU:O	1:D:366:LYS:HG3	2.14	0.47
1:B:45:GLY:HA2	1:B:73:GLN:HG2	1.94	0.47
1:C:40:LEU:HD12	1:C:320:ARG:HG2	1.95	0.47
1:F:390:ARG:NH1	1:F:394:ASP:OD1	2.36	0.47
1:C:270:ILE:HA	1:C:345:PHE:HZ	1.80	0.47
1:D:52:ILE:HD11	1:D:63:MET:HG2	1.95	0.47
1:F:189:GLU:CD	1:F:216:ASN:HD22	2.08	0.47
1:B:22:GLU:HG2	1:B:68:ARG:HE	1.80	0.47
1:C:221:GLN:HG2	1:C:236:LYS:HD2	1.96	0.47
1:D:110:PHE:CD2	1:D:111:LYS:HG2	2.49	0.47
1:F:167:LEU:HD11	1:F:201:ALA:HB1	1.96	0.47
1:H:33:PRO:HD2	1:H:320:ARG:NH1	2.29	0.47
1:C:22:GLU:HA	1:C:68:ARG:HH11	1.79	0.47
1:E:105:SER:HB2	1:E:109:TYR:CE2	2.50	0.47
1:E:170:ASN:OD1	1:E:172:LYS:HG2	2.14	0.47
1:C:437:ASP:OD1	1:C:439:ASP:OD1	2.32	0.47
1:E:207:ASP:OD1	1:E:207:ASP:N	2.44	0.47
1:G:313:GLY:O	1:G:314:ARG:NH1	2.45	0.47
1:H:254:LYS:NZ	1:H:259:ASP:O	2.46	0.47
1:A:444:GLU:HA	1:A:447:LEU:HG	1.97	0.47
1:B:223:ASN:HB3	1:B:231:LYS:HG2	1.96	0.47
1:C:318:THR:O	1:C:318:THR:HG23	2.15	0.47
1:D:313:GLY:O	1:D:314:ARG:NH1	2.48	0.47
1:E:111:LYS:NZ	1:E:151:GLU:HG2	2.29	0.47
1:C:204:VAL:O	1:C:205:ASN:HB3	2.15	0.47
1:E:149:ASP:OD1	1:E:151:GLU:HB3	2.15	0.47
1:B:274:THR:OG1	1:B:274:THR:O	2.29	0.47
1:E:313:GLY:O	1:E:314:ARG:NH1	2.46	0.47
1:H:57:ILE:HD13	1:H:64:ALA:CB	2.45	0.47
1:B:246:ARG:O	1:B:249:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ARG:O	1:C:249:SER:OG	2.19	0.46
1:G:67:SER:HB2	1:G:108:ASP:HB2	1.98	0.46
1:G:68:ARG:HH11	1:G:68:ARG:CB	2.27	0.46
1:B:29:SER:N	1:B:48:GLN:HE21	2.13	0.46
1:E:333:ARG:HD3	1:E:424:LEU:HD11	1.97	0.46
1:B:317:ASN:OD1	1:B:325:ARG:NH2	2.48	0.46
1:G:442:GLU:HA	1:G:445:ARG:HG3	1.96	0.46
1:G:23:HIS:CD2	1:G:68:ARG:HB3	2.50	0.46
1:H:263:PHE:CZ	1:H:303:ARG:NH1	2.83	0.46
1:C:384:LYS:O	1:C:388:ARG:NH1	2.43	0.46
1:C:385:THR:O	1:C:385:THR:CG2	2.64	0.46
1:C:390:ARG:HD2	1:C:390:ARG:HA	1.62	0.46
1:C:61:HIS:ND1	1:C:62:PRO:HD2	2.31	0.46
1:G:169:GLY:HA3	1:G:174:ASN:ND2	2.30	0.46
1:H:102:GLY:C	1:H:104:TRP:CZ3	2.88	0.46
1:H:214:ILE:O	1:H:242:MET:HG3	2.15	0.46
1:H:367:ASP:OD1	1:H:369:ASP:OD1	2.34	0.46
1:H:23:HIS:CE1	1:H:68:ARG:HD2	2.50	0.46
1:A:239:ASP:OD2	2:A:500:A5A:N	2.48	0.46
1:C:367:ASP:OD1	1:C:369:ASP:OD1	2.33	0.46
1:E:177:GLU:OE2	1:E:224:ARG:CZ	2.64	0.46
1:G:40:LEU:HD12	1:G:320:ARG:HG2	1.98	0.46
1:H:138:PHE:CZ	1:H:146:LEU:HD22	2.50	0.46
1:H:23:HIS:HA	1:H:68:ARG:HG2	1.97	0.46
1:G:382:PHE:CE2	1:G:386:LEU:HD13	2.51	0.46
1:H:45:GLY:HA2	1:H:73:GLN:HG2	1.97	0.46
1:F:131:GLU:HB3	1:F:165:LYS:HZ2	1.80	0.46
1:A:85:LEU:HD23	1:A:326:ARG:NH2	2.30	0.46
1:B:289:ASP:OD1	1:B:289:ASP:N	2.48	0.46
1:B:316:ASP:OD1	1:B:317:ASN:N	2.48	0.46
1:C:23:HIS:CE1	1:C:109:TYR:OH	2.69	0.46
1:C:15:ILE:HG13	1:C:16:ASP:H	1.79	0.46
1:G:326:ARG:HH21	1:G:330:ARG:HH22	1.63	0.46
1:G:330:ARG:HH21	1:G:423:ASP:HB2	1.81	0.46
1:A:45:GLY:HA2	1:A:73:GLN:HG2	1.97	0.46
1:C:22:GLU:O	1:C:68:ARG:HD2	2.16	0.46
1:D:31:THR:HG21	1:D:308:ALA:HA	1.98	0.46
1:F:222:TYR:C	1:F:233:LEU:HD13	2.35	0.46
1:G:137:TYR:O	1:G:174:ASN:ND2	2.49	0.46
1:C:153:LYS:HE3	1:C:154:GLN:HB2	1.98	0.45
1:H:249:SER:OG	1:H:257:ASN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:HD11	1:B:425:THR:HG23	1.98	0.45
1:C:113:LEU:HD23	1:C:117:MET:SD	2.56	0.45
1:G:403:SER:C	1:G:404:LYS:HD3	2.37	0.45
1:H:117:MET:CB	1:H:120:GLU:HB2	2.45	0.45
1:C:385:THR:CG2	1:C:418:TYR:O	2.60	0.45
1:D:442:GLU:O	1:D:446:LYS:HG3	2.15	0.45
1:F:135:VAL:HG23	1:F:153:LYS:HZ1	1.81	0.45
1:F:289:ASP:N	1:F:289:ASP:OD1	2.49	0.45
1:F:61:HIS:ND1	1:F:62:PRO:HD2	2.31	0.45
1:B:136:THR:OG1	1:B:189:GLU:HG3	2.15	0.45
1:C:223:ASN:CG	1:C:233:LEU:HD21	2.37	0.45
1:C:444:GLU:HA	1:C:447:LEU:HB3	1.98	0.45
1:D:154:GLN:HA	1:D:157:GLN:HG3	1.98	0.45
1:H:117:MET:CG	1:H:120:GLU:HB2	2.47	0.45
1:E:333:ARG:CD	1:E:424:LEU:HD11	2.46	0.45
1:E:45:GLY:HA2	1:E:73:GLN:HG2	1.98	0.45
1:F:110:PHE:C	1:F:238:ILE:HD11	2.37	0.45
1:G:110:PHE:C	1:G:238:ILE:HD11	2.36	0.45
1:H:444:GLU:O	1:H:448:ALA:N	2.48	0.45
1:C:23:HIS:HD2	1:C:104:TRP:H	1.65	0.45
1:E:444:GLU:O	1:E:447:LEU:HB3	2.17	0.45
1:D:10:ILE:HG12	1:D:248:VAL:HG22	1.98	0.45
1:D:223:ASN:HB2	1:D:233:LEU:HD21	1.99	0.45
1:H:46:MET:SD	1:H:176:TRP:HZ3	2.39	0.45
1:H:51:PRO:HB2	1:H:57:ILE:HG23	1.99	0.45
1:A:270:ILE:HA	1:A:345:PHE:HZ	1.82	0.45
1:B:444:GLU:HA	1:B:447:LEU:HG	1.99	0.45
1:G:10:ILE:HD11	1:G:251:LEU:CD1	2.41	0.45
1:H:102:GLY:HA2	1:H:240:THR:HG22	1.99	0.45
1:B:110:PHE:C	1:B:238:ILE:HD11	2.37	0.44
1:B:48:GLN:OE1	1:B:49:PHE:CE2	2.70	0.44
1:H:71:ASN:H	1:H:104:TRP:HZ3	1.64	0.44
1:F:246:ARG:O	1:F:249:SER:HB3	2.16	0.44
1:A:246:ARG:O	1:A:249:SER:HB3	2.17	0.44
1:D:92:VAL:CG1	1:D:256:SER:HA	2.47	0.44
1:A:170:ASN:HD22	1:A:172:LYS:HE3	1.82	0.44
1:A:177:GLU:OE2	1:A:224:ARG:NH1	2.51	0.44
1:D:393:LEU:HD11	1:D:425:THR:HG23	1.99	0.44
1:D:422:VAL:HG21	1:D:441:PHE:CE2	2.52	0.44
1:B:28:SER:CB	1:B:73:GLN:HA	2.48	0.44
1:C:14:PHE:CE2	1:C:101:LEU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:MET:C	1:C:65:LYS:N	2.71	0.44
1:H:71:ASN:N	1:H:104:TRP:CZ3	2.84	0.44
1:A:39:LEU:O	1:A:320:ARG:NH1	2.51	0.44
1:B:214:ILE:O	1:B:242:MET:HG3	2.17	0.44
1:E:61:HIS:CE1	1:E:63:MET:HG2	2.52	0.44
1:D:191:HIS:CD2	1:D:204:VAL:HG13	2.53	0.44
1:D:92:VAL:HG13	1:D:256:SER:HA	2.00	0.44
1:F:122:LEU:HB3	1:F:128:ILE:HG21	1.99	0.44
1:F:135:VAL:HG23	1:F:153:LYS:NZ	2.32	0.44
1:F:138:PHE:CZ	1:F:171:MET:HE3	2.53	0.44
1:H:141:ASP:HB3	1:H:146:LEU:HD21	2.00	0.44
1:C:328:LEU:HD22	1:C:378:GLU:HB3	1.99	0.44
1:E:246:ARG:O	1:E:249:SER:HB3	2.17	0.44
1:F:138:PHE:HZ	1:F:171:MET:HE3	1.82	0.44
1:G:397:ILE:HD13	1:G:432:LYS:HD3	1.99	0.44
1:H:15:ILE:HG13	1:H:16:ASP:N	2.33	0.44
1:A:384:LYS:CE	1:B:409:ASP:OD2	2.66	0.44
1:B:55:ASN:O	1:E:154:GLN:NE2	2.51	0.44
1:H:146:LEU:C	1:H:146:LEU:HD12	2.39	0.44
1:A:105:SER:HB2	1:A:109:TYR:CE2	2.52	0.43
1:A:359:ASP:OD1	1:A:360:ALA:N	2.49	0.43
1:E:112:GLU:HG3	1:E:155:ILE:CD1	2.48	0.43
1:B:223:ASN:HD22	1:B:231:LYS:HE3	1.82	0.43
1:B:31:THR:HG21	1:B:308:ALA:HA	2.00	0.43
1:C:58:ASP:OD1	1:C:59:PRO:HD2	2.18	0.43
1:D:326:ARG:HG2	1:D:421:PRO:HB3	2.00	0.43
1:F:282:LYS:N	1:F:292:ASP:OD2	2.47	0.43
1:G:105:SER:HB2	1:G:109:TYR:CE2	2.54	0.43
1:G:337:GLU:OE2	1:G:390:ARG:HG3	2.18	0.43
1:B:105:SER:HB2	1:B:109:TYR:CE2	2.52	0.43
1:B:92:VAL:CG1	1:B:256:SER:HA	2.48	0.43
1:C:337:GLU:CD	1:C:390:ARG:HH11	2.22	0.43
1:F:45:GLY:HA2	1:F:73:GLN:HG2	2.00	0.43
1:C:92:VAL:CG1	1:C:256:SER:HA	2.48	0.43
1:G:224:ARG:NH2	1:G:230:LEU:HD11	2.33	0.43
1:H:146:LEU:HB2	1:H:147:GLU:H	1.52	0.43
1:B:230:LEU:HD23	1:B:230:LEU:HA	1.70	0.43
1:D:422:VAL:CG2	1:D:441:PHE:CZ	3.01	0.43
1:F:153:LYS:HA	1:F:153:LYS:HD2	1.09	0.43
1:G:326:ARG:HG2	1:G:421:PRO:HB3	1.99	0.43
1:B:254:LYS:NZ	1:B:259:ASP:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LEU:HA	1:E:40:LEU:HD12	1.73	0.43
1:E:80:GLY:N	1:E:83:ASN:HB2	2.33	0.43
1:F:35:ASP:CG	1:H:278:PRO:HD2	2.39	0.43
1:H:246:ARG:HG3	1:H:257:ASN:HD21	1.84	0.43
1:D:27:HIS:HD2	1:D:28:SER:H	1.64	0.43
1:F:35:ASP:OD2	1:H:277:ARG:HA	2.18	0.43
1:E:110:PHE:C	1:E:238:ILE:HD11	2.39	0.43
1:E:61:HIS:ND1	1:E:62:PRO:HD2	2.34	0.43
1:G:18:PHE:O	1:G:23:HIS:N	2.33	0.43
1:B:128:ILE:HD12	1:B:128:ILE:C	2.38	0.43
1:C:319:GLY:O	1:C:323:VAL:HG23	2.19	0.43
1:E:61:HIS:ND1	1:E:63:MET:HG2	2.33	0.43
1:F:110:PHE:CE1	1:F:236:LYS:HB3	2.54	0.43
1:F:316:ASP:OD1	1:F:317:ASN:N	2.52	0.43
1:D:104:TRP:CD1	1:D:239:ASP:HA	2.54	0.43
1:E:35:ASP:HB2	1:G:277:ARG:HB2	2.01	0.43
1:C:22:GLU:HG3	1:C:22:GLU:H	1.53	0.42
1:D:424:LEU:HD12	1:D:427:LEU:HD12	2.01	0.42
1:F:110:PHE:HZ	1:F:221:GLN:HE21	1.66	0.42
1:G:37:PRO:HA	1:G:320:ARG:HH22	1.84	0.42
1:H:117:MET:C	1:H:119:LEU:N	2.71	0.42
1:B:162:ASP:OD2	1:B:164:THR:OG1	2.24	0.42
1:C:67:SER:HA	1:C:106:PHE:HB2	2.01	0.42
1:F:104:TRP:CD1	1:F:239:ASP:HA	2.54	0.42
1:H:150:LEU:HA	1:H:153:LYS:HB3	1.99	0.42
1:H:18:PHE:O	1:H:23:HIS:ND1	2.47	0.42
1:H:33:PRO:HD2	1:H:320:ARG:HH22	1.84	0.42
1:B:231:LYS:HD2	1:B:233:LEU:HD23	2.01	0.42
1:B:92:VAL:HG13	1:B:256:SER:HA	2.01	0.42
1:B:35:ASP:HB2	1:C:277:ARG:HB2	2.00	0.42
1:F:225:GLU:OE2	1:F:231:LYS:HB2	2.19	0.42
1:D:107:GLY:HA2	1:D:235:LYS:HG3	2.01	0.42
1:G:169:GLY:HA3	1:G:174:ASN:HD22	1.84	0.42
1:H:270:ILE:HA	1:H:345:PHE:CZ	2.52	0.42
1:G:270:ILE:HA	1:G:345:PHE:HZ	1.84	0.42
1:H:93:TYR:CE2	1:H:94:HIS:CE1	3.07	0.42
1:B:111:LYS:NZ	1:B:149:ASP:OD1	2.53	0.42
1:C:103:SER:O	1:C:240:THR:HB	2.19	0.42
1:C:385:THR:CG2	1:C:418:TYR:HB3	2.49	0.42
1:H:110:PHE:CG	1:H:111:LYS:N	2.85	0.42
1:H:277:ARG:HH22	1:H:280:THR:CG2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLN:HG3	1:B:48:GLN:H	1.66	0.42
1:C:204:VAL:O	1:C:205:ASN:CB	2.68	0.42
1:E:446:LYS:NZ	1:E:450:LEU:HD11	2.35	0.42
1:B:67:SER:HB2	1:B:108:ASP:HB2	2.01	0.42
1:B:282:LYS:HD2	1:B:287:ASP:OD1	2.19	0.42
1:C:22:GLU:HA	1:C:68:ARG:HD2	2.01	0.42
1:D:19:LYS:HA	1:D:23:HIS:H	1.85	0.42
1:H:105:SER:HB2	1:H:109:TYR:CE2	2.54	0.42
1:B:336:HIS:ND1	1:B:341:ALA:O	2.51	0.42
1:C:111:LYS:NZ	1:C:149:ASP:OD2	2.48	0.42
1:C:304:THR:HG1	1:C:305:ILE:H	1.67	0.42
1:C:413:LEU:HD12	1:C:417:THR:OG1	2.20	0.42
1:H:177:GLU:HG2	1:H:184:CYS:CB	2.49	0.42
1:A:172:LYS:HG3	1:A:173:ASP:N	2.35	0.42
1:B:177:GLU:HG2	1:B:184:CYS:CB	2.50	0.42
1:F:131:GLU:HB3	1:F:165:LYS:HE3	2.02	0.42
1:F:137:TYR:CD2	1:F:153:LYS:HE2	2.55	0.42
1:B:153:LYS:HD3	1:B:166:ILE:HG21	2.00	0.41
1:B:222:TYR:HD1	1:B:231:LYS:O	2.02	0.41
1:C:316:ASP:CG	1:C:318:THR:HG22	2.41	0.41
1:D:390:ARG:HG3	1:D:390:ARG:HH11	1.84	0.41
1:E:150:LEU:HD23	1:E:153:LYS:HD2	2.02	0.41
1:A:153:LYS:O	1:A:157:GLN:HG3	2.19	0.41
1:C:386:LEU:O	1:C:390:ARG:HG2	2.20	0.41
1:G:77:ARG:HD3	1:G:82:HIS:HB3	2.02	0.41
1:B:109:TYR:CE1	1:B:238:ILE:HD12	2.55	0.41
1:E:39:LEU:HD21	1:E:47:ASN:OD1	2.20	0.41
1:G:93:TYR:CE2	1:G:94:HIS:CE1	3.08	0.41
1:H:194:ARG:HH12	1:H:249:SER:HB3	1.86	0.41
1:F:62:PRO:HD3	1:H:340:ASN:OD1	2.20	0.41
1:E:109:TYR:CE1	1:E:238:ILE:HD12	2.55	0.41
1:E:390:ARG:NH1	1:E:428:ILE:HG21	2.36	0.41
1:G:22:GLU:HB3	1:G:68:ARG:HD2	2.01	0.41
1:A:75:CYS:O	1:A:97:PHE:HA	2.21	0.41
1:C:113:LEU:HD21	1:C:117:MET:HE1	2.01	0.41
1:D:15:ILE:HD12	1:D:25:TYR:CD1	2.55	0.41
1:D:61:HIS:ND1	1:D:62:PRO:HD2	2.35	0.41
1:E:13:ARG:CZ	1:E:20:ARG:HH12	2.33	0.41
1:E:35:ASP:CG	1:G:278:PRO:HD2	2.40	0.41
1:G:19:LYS:HD3	1:G:24:THR:HA	2.02	0.41
1:G:80:GLY:HA2	1:G:81:LYS:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:VAL:CG1	1:E:256:SER:HA	2.51	0.41
1:C:93:TYR:CE2	1:C:94:HIS:CE1	3.09	0.41
1:H:117:MET:CA	1:H:119:LEU:H	2.33	0.41
1:H:409:ASP:N	1:H:409:ASP:OD1	2.53	0.41
1:C:92:VAL:HG13	1:C:256:SER:HA	2.03	0.41
1:E:390:ARG:HH12	1:E:432:LYS:HE2	1.84	0.41
1:F:103:SER:O	1:F:240:THR:HB	2.21	0.41
1:H:413:LEU:HD12	1:H:417:THR:OG1	2.21	0.41
1:A:122:LEU:C	1:A:128:ILE:HG22	2.42	0.41
1:B:109:TYR:CD1	1:B:238:ILE:HD12	2.56	0.41
1:B:113:LEU:O	1:B:117:MET:HG3	2.21	0.41
1:C:295:TYR:HD1	1:C:339:LEU:HD21	1.85	0.41
1:D:27:HIS:HD2	1:D:28:SER:N	2.18	0.41
1:F:131:GLU:HB3	1:F:165:LYS:NZ	2.35	0.41
1:H:52:ILE:HD11	1:H:63:MET:HG2	2.02	0.41
1:B:59:PRO:HG2	1:E:150:LEU:HB2	2.02	0.41
1:C:277:ARG:HH12	1:C:289:ASP:CG	2.24	0.41
1:E:85:LEU:HD23	1:E:326:ARG:NH2	2.36	0.41
1:A:109:TYR:CE1	1:A:238:ILE:HD12	2.56	0.41
1:F:113:LEU:O	1:F:117:MET:HG3	2.21	0.41
1:A:113:LEU:O	1:A:117:MET:HG3	2.22	0.40
1:C:111:LYS:NZ	1:C:149:ASP:CG	2.75	0.40
1:D:19:LYS:HA	1:D:23:HIS:N	2.36	0.40
1:A:23:HIS:CD2	1:A:68:ARG:HB2	2.56	0.40
1:A:434:LEU:HD12	1:A:434:LEU:N	2.36	0.40
1:F:80:GLY:N	1:F:83:ASN:HB2	2.36	0.40
1:G:330:ARG:HD2	1:G:330:ARG:HH11	1.68	0.40
1:C:104:TRP:CD1	1:C:239:ASP:HA	2.56	0.40
1:D:270:ILE:HA	1:D:345:PHE:HZ	1.86	0.40
1:B:61:HIS:ND1	1:B:62:PRO:HD2	2.36	0.40
1:C:137:TYR:CA	1:C:174:ASN:HD22	2.34	0.40
1:G:14:PHE:CE1	1:G:18:PHE:HE2	2.40	0.40
1:C:300:ASP:C	1:C:300:ASP:OD1	2.60	0.40
1:C:97:PHE:CB	1:C:304:THR:HG22	2.52	0.40
1:D:80:GLY:N	1:D:83:ASN:HB2	2.37	0.40
1:E:113:LEU:O	1:E:117:MET:HG3	2.22	0.40
1:G:245:GLU:HG3	1:G:262:LEU:HD13	2.02	0.40

All (4) 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:377:GLU:OE1	1:F:395:ARG:NH1[1_546]	1.89	0.31
1:A:154:GLN:NE2	1:F:55:ASN:O[1_545]	2.10	0.10
1:E:445:ARG:NE	1:G:405:THR:OG1[1_655]	2.12	0.08
1:D:388:ARG:NH2	1:H:366:LYS:O[1_645]	2.15	0.05

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	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	52	79
1	B	448/450 (100%)	431 (96%)	12 (3%)	5 (1%)	17	40
1	C	442/450 (98%)	426 (96%)	12 (3%)	4 (1%)	21	46
1	D	445/450 (99%)	431 (97%)	14 (3%)	0	100	100
1	E	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	52	79
1	F	447/450 (99%)	434 (97%)	11 (2%)	2 (0%)	39	67
1	G	447/450 (99%)	429 (96%)	15 (3%)	3 (1%)	26	53
1	H	444/450 (99%)	421 (95%)	18 (4%)	5 (1%)	17	40
All	All	3569/3600 (99%)	3444 (96%)	104 (3%)	21 (1%)	30	56

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	B	37	PRO
1	C	22	GLU
1	F	37	PRO
1	H	37	PRO
1	H	103	SER
1	H	104	TRP
1	C	158	ASN
1	G	37	PRO

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Mol	Chain	Res	Type
1	H	142	GLU
1	B	275	GLY
1	B	35	ASP
1	G	22	GLU
1	C	35	ASP
1	B	278	PRO
1	C	59	PRO
1	B	36	ASP
1	E	36	ASP
1	F	36	ASP
1	G	36	ASP
1	H	36	ASP

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	379/379 (100%)	360 (95%)	19 (5%)	30	57
1	B	379/379 (100%)	358 (94%)	21 (6%)	27	52
1	C	374/379 (99%)	355 (95%)	19 (5%)	29	56
1	D	376/379 (99%)	357 (95%)	19 (5%)	29	56
1	E	379/379 (100%)	363 (96%)	16 (4%)	36	65
1	F	378/379 (100%)	362 (96%)	16 (4%)	36	65
1	G	378/379 (100%)	361 (96%)	17 (4%)	34	62
1	H	375/379 (99%)	353 (94%)	22 (6%)	24	49
All	All	3018/3032 (100%)	2869 (95%)	149 (5%)	31	58

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	29	SER
1	A	31	THR

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Mol	Chain	Res	Type
1	A	40	LEU
1	A	46	MET
1	A	55	ASN
1	A	60	SER
1	A	68	ARG
1	A	131	GLU
1	A	147	GLU
1	A	283	VAL
1	A	301	HIS
1	A	355	GLN
1	A	395	ARG
1	A	402	ASP
1	A	403	SER
1	A	423	ASP
1	A	443	GLU
1	A	453	GLN
1	B	4	THR
1	B	22	GLU
1	B	31	THR
1	B	46	MET
1	B	48	GLN
1	B	92	VAL
1	B	121	LEU
1	B	150	LEU
1	B	153	LYS
1	B	178	MET
1	B	198	ARG
1	B	230	LEU
1	B	282	LYS
1	B	283	VAL
1	B	303	ARG
1	B	328	LEU
1	B	399	SER
1	B	413	LEU
1	B	422	VAL
1	B	423	ASP
1	B	439	ASP
1	C	4	THR
1	C	12	GLN
1	C	19	LYS
1	C	56	THR
1	C	60	SER

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Mol	Chain	Res	Type
1	C	81	LYS
1	C	88	VAL
1	C	92	VAL
1	C	113	LEU
1	C	150	LEU
1	C	178	MET
1	C	227	ASP
1	C	303	ARG
1	C	363	GLU
1	C	369	ASP
1	C	390	ARG
1	C	399	SER
1	C	423	ASP
1	C	443	GLU
1	D	5	LEU
1	D	9	GLU
1	D	10	ILE
1	D	15	ILE
1	D	31	THR
1	D	46	MET
1	D	47	ASN
1	D	88	VAL
1	D	92	VAL
1	D	113	LEU
1	D	150	LEU
1	D	171	MET
1	D	178	MET
1	D	283	VAL
1	D	301	HIS
1	D	306	THR
1	D	390	ARG
1	D	399	SER
1	D	423	ASP
1	E	4	THR
1	E	29	SER
1	E	88	VAL
1	E	92	VAL
1	E	151	GLU
1	E	155	ILE
1	E	178	MET
1	E	221	GLN
1	E	233	LEU

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Mol	Chain	Res	Type
1	E	283	VAL
1	E	303	ARG
1	E	328	LEU
1	E	384	LYS
1	E	399	SER
1	E	423	ASP
1	E	445	ARG
1	F	29	SER
1	F	46	MET
1	F	60	SER
1	F	88	VAL
1	F	108	ASP
1	F	150	LEU
1	F	189	GLU
1	F	207	ASP
1	F	227	ASP
1	F	283	VAL
1	F	301	HIS
1	F	303	ARG
1	F	328	LEU
1	F	403	SER
1	F	423	ASP
1	F	443	GLU
1	G	11	ARG
1	G	19	LYS
1	G	29	SER
1	G	31	THR
1	G	55	ASN
1	G	94	HIS
1	G	113	LEU
1	G	131	GLU
1	G	178	MET
1	G	198	ARG
1	G	301	HIS
1	G	303	ARG
1	G	328	LEU
1	G	365	LYS
1	G	399	SER
1	G	422	VAL
1	G	423	ASP
1	H	4	THR
1	H	29	SER

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Mol	Chain	Res	Type
1	H	81	LYS
1	H	88	VAL
1	H	104	TRP
1	H	116	LYS
1	H	120	GLU
1	H	146	LEU
1	H	153	LYS
1	H	154	GLN
1	H	230	LEU
1	H	236	LYS
1	H	249	SER
1	H	301	HIS
1	H	326	ARG
1	H	328	LEU
1	H	370	MET
1	H	386	LEU
1	H	388	ARG
1	H	423	ASP
1	H	439	ASP
1	H	442	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	205	ASN
1	B	48	GLN
1	C	154	GLN
1	C	174	ASN
1	C	205	ASN
1	C	223	ASN
1	D	27	HIS
1	D	47	ASN
1	D	174	ASN
1	D	191	HIS
1	D	340	ASN
1	E	94	HIS
1	E	154	GLN
1	E	205	ASN
1	E	301	HIS
1	G	55	ASN
1	G	124	GLN

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Mol	Chain	Res	Type
1	G	174	ASN
1	G	223	ASN
1	G	340	ASN
1	G	355	GLN
1	H	157	GLN
1	H	257	ASN
1	H	340	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A5A	A	500	-	26,30,30	1.76	5 (19%)	27,45,45	2.60	10 (37%)
2	A5A	B	500	-	26,30,30	1.90	4 (15%)	27,45,45	2.51	6 (22%)
2	A5A	C	500	-	26,30,30	2.11	6 (23%)	27,45,45	2.34	8 (29%)
2	A5A	D	500	-	26,30,30	1.47	4 (15%)	27,45,45	2.56	7 (25%)
2	A5A	E	500	-	26,30,30	1.55	5 (19%)	27,45,45	2.22	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A5A	F	500	-	26,30,30	2.21	5 (19%)	27,45,45	2.43	7 (25%)
2	A5A	G	500	-	26,30,30	1.50	5 (19%)	27,45,45	1.88	5 (18%)
2	A5A	H	500	-	26,30,30	1.51	6 (23%)	27,45,45	1.72	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A5A	A	500	-	-	0/14/35/35	0/3/3/3
2	A5A	B	500	-	-	0/14/35/35	0/3/3/3
2	A5A	C	500	-	-	0/14/35/35	0/3/3/3
2	A5A	D	500	-	-	0/14/35/35	0/3/3/3
2	A5A	E	500	-	-	0/14/35/35	0/3/3/3
2	A5A	F	500	-	-	0/14/35/35	0/3/3/3
2	A5A	G	500	-	-	0/14/35/35	0/3/3/3
2	A5A	H	500	-	-	0/14/35/35	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	A5A	O5'-S	-6.12	1.50	1.59
2	B	500	A5A	O5'-S	-5.41	1.51	1.59
2	A	500	A5A	O5'-S	-5.18	1.51	1.59
2	F	500	A5A	O5'-S	-4.76	1.52	1.59
2	G	500	A5A	O5'-S	-3.26	1.54	1.59
2	H	500	A5A	O5'-S	-3.25	1.54	1.59
2	E	500	A5A	O5'-S	-3.16	1.54	1.59
2	D	500	A5A	O5'-S	-3.08	1.54	1.59
2	G	500	A5A	C2'-C1'	-2.99	1.48	1.53
2	H	500	A5A	C2'-C1'	-2.64	1.49	1.53
2	A	500	A5A	C2'-C1'	-2.39	1.49	1.53
2	C	500	A5A	C2'-C1'	-2.30	1.50	1.53
2	G	500	A5A	C-N3S	-2.22	1.34	1.37
2	A	500	A5A	S-N3S	2.05	1.62	1.60
2	E	500	A5A	O1S-S	2.24	1.44	1.42
2	A	500	A5A	C5-C4	2.25	1.45	1.40
2	E	500	A5A	S-N3S	2.26	1.62	1.60
2	B	500	A5A	C5-C4	2.38	1.45	1.40
2	E	500	A5A	C5-C4	2.50	1.46	1.40
2	H	500	A5A	O2S-S	2.50	1.44	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	A5A	S-N3S	2.59	1.62	1.60
2	H	500	A5A	C5-C4	2.62	1.46	1.40
2	G	500	A5A	C5-C4	2.68	1.46	1.40
2	H	500	A5A	O4'-C1'	2.70	1.45	1.41
2	D	500	A5A	C5-C4	2.72	1.46	1.40
2	G	500	A5A	O2S-S	2.76	1.44	1.42
2	B	500	A5A	S-N3S	2.83	1.63	1.60
2	D	500	A5A	S-N3S	2.89	1.63	1.60
2	D	500	A5A	O2S-S	3.16	1.45	1.42
2	C	500	A5A	O2S-S	3.23	1.45	1.42
2	F	500	A5A	S-N3S	3.35	1.63	1.60
2	C	500	A5A	C5-C4	3.35	1.48	1.40
2	F	500	A5A	C5-C4	3.57	1.48	1.40
2	C	500	A5A	O1S-S	3.59	1.45	1.42
2	E	500	A5A	O2S-S	3.87	1.45	1.42
2	C	500	A5A	S-N3S	3.87	1.64	1.60
2	A	500	A5A	O2S-S	4.71	1.46	1.42
2	B	500	A5A	O2S-S	4.73	1.46	1.42
2	F	500	A5A	O2S-S	4.79	1.46	1.42
2	F	500	A5A	O1S-S	5.94	1.47	1.42

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	A5A	N3-C2-N1	-10.17	120.88	128.87
2	D	500	A5A	N3-C2-N1	-9.59	121.34	128.87
2	B	500	A5A	N3-C2-N1	-9.16	121.67	128.87
2	F	500	A5A	N3-C2-N1	-7.45	123.02	128.87
2	H	500	A5A	N3-C2-N1	-6.75	123.56	128.87
2	C	500	A5A	N3-C2-N1	-6.63	123.66	128.87
2	G	500	A5A	N3-C2-N1	-6.51	123.76	128.87
2	E	500	A5A	N3-C2-N1	-6.37	123.86	128.87
2	D	500	A5A	C1'-N9-C4	-5.29	120.91	126.81
2	B	500	A5A	C2'-C1'-N9	-4.65	101.01	113.47
2	C	500	A5A	C-N3S-S	-4.65	118.66	124.22
2	C	500	A5A	C1'-N9-C4	-4.04	122.30	126.81
2	E	500	A5A	C2'-C1'-N9	-4.01	102.72	113.47
2	F	500	A5A	C2'-C1'-N9	-3.92	102.98	113.47
2	B	500	A5A	O-C-N3S	-3.62	117.36	121.59
2	F	500	A5A	C4'-O4'-C1'	-3.61	105.81	109.64
2	G	500	A5A	C1'-N9-C4	-3.57	122.82	126.81
2	D	500	A5A	C2'-C1'-N9	-3.24	104.81	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	500	A5A	C2'-C1'-N9	-3.00	105.44	113.47
2	A	500	A5A	C1'-N9-C4	-2.78	123.70	126.81
2	H	500	A5A	C2'-C1'-N9	-2.75	106.11	113.47
2	F	500	A5A	C-N3S-S	-2.52	121.21	124.22
2	G	500	A5A	C-N3S-S	-2.45	121.29	124.22
2	H	500	A5A	C1'-N9-C4	-2.38	124.15	126.81
2	A	500	A5A	O3'-C3'-C2'	-2.30	104.42	111.86
2	A	500	A5A	O4'-C4'-C3'	-2.28	100.54	105.16
2	E	500	A5A	C1'-N9-C4	-2.12	124.44	126.81
2	D	500	A5A	O5'-C5'-C4'	2.07	111.97	107.96
2	A	500	A5A	C2'-C3'-C4'	2.19	107.13	102.64
2	E	500	A5A	O4'-C1'-N9	2.21	112.28	108.11
2	A	500	A5A	C2-N1-C6	2.25	122.78	118.77
2	D	500	A5A	C2-N1-C6	2.25	122.79	118.77
2	H	500	A5A	C-N3S-S	2.28	126.94	124.22
2	G	500	A5A	O5'-S-O1S	2.28	113.02	105.66
2	C	500	A5A	O1S-S-N3S	2.32	111.80	108.58
2	B	500	A5A	O5'-S-O2S	2.49	113.69	105.66
2	C	500	A5A	O5'-S-O1S	2.52	113.79	105.66
2	A	500	A5A	C4'-O4'-C1'	2.54	112.33	109.64
2	D	500	A5A	CA-C-N3S	2.56	122.01	115.48
2	F	500	A5A	O1S-S-N3S	2.58	112.16	108.58
2	D	500	A5A	O4'-C1'-N9	2.63	113.08	108.11
2	A	500	A5A	O2S-S-N3S	2.67	112.28	108.58
2	A	500	A5A	O1S-S-N3S	2.74	112.38	108.58
2	C	500	A5A	C2-N1-C6	2.80	123.76	118.77
2	B	500	A5A	O2S-S-N3S	2.91	112.61	108.58
2	A	500	A5A	O5'-S-O1S	2.95	115.18	105.66
2	C	500	A5A	CA-C-N3S	3.19	123.63	115.48
2	E	500	A5A	O-C-N3S	3.25	125.39	121.59
2	F	500	A5A	C2'-C3'-C4'	3.31	109.41	102.64
2	B	500	A5A	C2'-C3'-C4'	3.61	110.01	102.64
2	E	500	A5A	C-N3S-S	4.05	129.06	124.22
2	C	500	A5A	O2S-S-N3S	4.13	114.31	108.58
2	E	500	A5A	O1S-S-N3S	4.16	114.35	108.58
2	F	500	A5A	O2S-S-N3S	4.20	114.40	108.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	A5A	1	0
2	C	500	A5A	3	0
2	D	500	A5A	1	0
2	E	500	A5A	2	0

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	450/450 (100%)	1.13	80 (17%) 2 1	19, 47, 69, 87	0
1	B	450/450 (100%)	1.43	105 (23%) 1 1	22, 48, 86, 113	0
1	C	444/450 (98%)	1.57	128 (28%) 1 0	34, 63, 92, 124	0
1	D	447/450 (99%)	1.70	131 (29%) 1 0	19, 61, 89, 127	0
1	E	450/450 (100%)	1.19	85 (18%) 2 1	21, 48, 75, 90	0
1	F	449/450 (99%)	1.23	91 (20%) 1 1	19, 46, 81, 100	0
1	G	449/450 (99%)	1.52	121 (26%) 1 0	31, 59, 85, 109	0
1	H	446/450 (99%)	1.54	131 (29%) 1 0	29, 60, 101, 122	0
All	All	3585/3600 (99%)	1.41	872 (24%) 1 1	19, 54, 88, 127	0

All (872) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	GLY	14.7
1	D	237	SER	13.8
1	E	288	ALA	11.0
1	G	122	LEU	10.3
1	H	237	SER	10.3
1	C	25	TYR	10.1
1	B	118	ALA	10.0
1	B	204	VAL	9.7
1	D	69	ALA	9.5
1	G	66	LEU	9.2
1	B	156	TRP	9.2
1	C	65	LYS	8.8
1	F	148	ALA	8.6
1	D	96	THR	8.5
1	F	192	TYR	8.4
1	D	243	GLY	8.3

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Mol	Chain	Res	Type	RSRZ
1	G	5	LEU	8.3
1	B	168	PRO	8.2
1	C	106	PHE	8.0
1	D	119	LEU	7.9
1	G	53	PHE	7.8
1	D	220	ILE	7.7
1	E	35	ASP	7.4
1	B	230	LEU	7.2
1	H	103	SER	7.0
1	B	143	ALA	7.0
1	D	114	ALA	7.0
1	C	217	LEU	7.0
1	F	205	ASN	6.9
1	H	30	ALA	6.8
1	H	445	ARG	6.8
1	E	38	THR	6.8
1	D	48	GLN	6.8
1	G	176	TRP	6.8
1	G	144	ALA	6.7
1	G	119	LEU	6.7
1	F	92	VAL	6.6
1	H	115	CYS	6.6
1	H	162	ASP	6.6
1	G	57	ILE	6.6
1	H	152	CYS	6.6
1	E	128	ILE	6.5
1	G	185	GLY	6.5
1	B	397	ILE	6.5
1	B	251	LEU	6.5
1	E	175	PHE	6.4
1	C	390	ARG	6.4
1	D	111	LYS	6.4
1	A	277	ARG	6.4
1	G	284	GLY	6.3
1	D	176	TRP	6.3
1	C	270	ILE	6.3
1	E	129	PRO	6.2
1	C	156	TRP	6.2
1	D	133	LEU	6.2
1	F	133	LEU	6.2
1	D	15	ILE	6.2
1	H	310	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	183	PRO	6.2
1	D	236	LYS	6.1
1	H	92	VAL	6.1
1	H	59	PRO	6.1
1	G	299	ALA	6.1
1	F	116	LYS	6.0
1	G	160	GLY	6.0
1	F	118	ALA	6.0
1	D	192	TYR	6.0
1	H	299	ALA	5.9
1	C	118	ALA	5.9
1	A	112	GLU	5.8
1	D	134	TYR	5.8
1	C	219	PHE	5.8
1	C	29	SER	5.7
1	H	150	LEU	5.7
1	F	119	LEU	5.7
1	G	171	MET	5.7
1	C	172	LYS	5.7
1	D	346	PHE	5.6
1	H	260	THR	5.6
1	D	217	LEU	5.5
1	C	152	CYS	5.5
1	B	147	GLU	5.5
1	D	141	ASP	5.5
1	F	117	MET	5.4
1	H	183	PRO	5.4
1	G	345	PHE	5.4
1	H	200	ALA	5.4
1	F	33	PRO	5.4
1	A	252	GLN	5.4
1	B	130	ILE	5.4
1	D	14	PHE	5.4
1	E	183	PRO	5.3
1	H	57	ILE	5.3
1	A	17	PHE	5.3
1	F	86	ASP	5.3
1	A	421	PRO	5.3
1	H	78	ALA	5.3
1	G	121	LEU	5.2
1	B	153	LYS	5.2
1	D	191	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	H	443	GLU	5.2
1	D	68	ARG	5.2
1	F	135	VAL	5.2
1	G	134	TYR	5.2
1	E	233	LEU	5.2
1	G	244	LEU	5.2
1	D	242	MET	5.2
1	F	436	VAL	5.2
1	D	238	ILE	5.1
1	H	65	LYS	5.1
1	G	347	ALA	5.1
1	G	81	LYS	5.1
1	G	266	TYR	5.1
1	B	84	ASP	5.1
1	D	171	MET	5.0
1	B	201	ALA	5.0
1	D	214	ILE	5.0
1	C	44	ALA	5.0
1	B	152	CYS	5.0
1	C	258	TYR	5.0
1	D	418	TYR	5.0
1	D	231	LYS	4.9
1	G	33	PRO	4.9
1	F	225	GLU	4.9
1	H	161	LEU	4.9
1	B	386	LEU	4.8
1	C	70	ALA	4.8
1	D	257	ASN	4.8
1	B	203	LEU	4.8
1	E	44	ALA	4.7
1	B	26	VAL	4.7
1	B	86	ASP	4.7
1	H	23	HIS	4.7
1	C	64	ALA	4.7
1	A	137	TYR	4.7
1	D	130	ILE	4.7
1	C	137	TYR	4.6
1	B	42	ALA	4.6
1	D	414	LEU	4.6
1	H	54	LEU	4.6
1	C	421	PRO	4.6
1	D	89	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	59	PRO	4.6
1	D	112	GLU	4.6
1	E	429	ALA	4.6
1	A	339	LEU	4.6
1	E	230	LEU	4.6
1	H	43	ASN	4.6
1	E	10	ILE	4.6
1	F	107	GLY	4.6
1	C	224	ARG	4.5
1	G	175	PHE	4.5
1	B	443	GLU	4.5
1	E	212	LEU	4.5
1	C	220	ILE	4.5
1	C	21	ASN	4.5
1	D	295	TYR	4.5
1	B	148	ALA	4.5
1	E	302	ALA	4.5
1	F	235	LYS	4.5
1	C	15	ILE	4.4
1	F	299	ALA	4.4
1	G	389	GLY	4.4
1	G	357	LEU	4.4
1	C	41	PHE	4.4
1	H	73	GLN	4.4
1	D	80	GLY	4.4
1	F	87	ASP	4.4
1	G	15	ILE	4.4
1	A	334	TYR	4.4
1	C	84	ASP	4.4
1	H	96	THR	4.4
1	H	143	ALA	4.4
1	D	32	ILE	4.3
1	A	200	ALA	4.3
1	D	152	CYS	4.3
1	C	66	LEU	4.3
1	A	341	ALA	4.3
1	D	235	LYS	4.3
1	D	51	PRO	4.3
1	D	160	GLY	4.3
1	D	136	THR	4.3
1	D	369	ASP	4.3
1	F	154	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	67	SER	4.3
1	A	371	VAL	4.2
1	G	214	ILE	4.2
1	H	229	ILE	4.2
1	C	362	PRO	4.2
1	H	244	LEU	4.2
1	E	370	MET	4.2
1	B	200	ALA	4.2
1	A	328	LEU	4.2
1	H	77	ARG	4.2
1	H	187	CYS	4.2
1	C	229	ILE	4.2
1	F	179	GLY	4.2
1	B	144	ALA	4.2
1	C	43	ASN	4.2
1	H	324	LEU	4.2
1	B	226	ALA	4.2
1	C	349	LEU	4.1
1	C	170	ASN	4.1
1	G	448	ALA	4.1
1	C	274	THR	4.1
1	F	138	PHE	4.1
1	F	137	TYR	4.1
1	E	78	ALA	4.1
1	D	417	THR	4.1
1	B	41	PHE	4.1
1	D	199	ASP	4.1
1	G	205	ASN	4.1
1	G	126	PHE	4.1
1	B	339	LEU	4.1
1	C	386	LEU	4.1
1	C	81	LYS	4.1
1	C	5	LEU	4.0
1	E	410	THR	4.0
1	F	220	ILE	4.0
1	H	50	LYS	4.0
1	G	96	THR	4.0
1	D	450	LEU	4.0
1	H	60	SER	4.0
1	E	297	VAL	4.0
1	B	137	TYR	4.0
1	D	49	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	123	THR	4.0
1	C	311	ASP	4.0
1	C	397	ILE	4.0
1	E	164	THR	3.9
1	E	57	ILE	3.9
1	G	392	ILE	3.9
1	B	32	ILE	3.9
1	B	36	ASP	3.9
1	E	79	GLY	3.9
1	E	30	ALA	3.9
1	G	73	GLN	3.9
1	D	121	LEU	3.9
1	C	100	MET	3.9
1	E	214	ILE	3.9
1	F	115	CYS	3.9
1	G	143	ALA	3.9
1	H	283	VAL	3.9
1	B	313	GLY	3.9
1	D	186	PRO	3.9
1	B	154	GLN	3.9
1	H	36	ASP	3.9
1	C	45	GLY	3.8
1	F	243	GLY	3.8
1	C	350	VAL	3.8
1	F	306	THR	3.8
1	D	361	PHE	3.8
1	B	197	GLY	3.8
1	E	186	PRO	3.8
1	C	30	ALA	3.8
1	H	153	LYS	3.8
1	C	82	HIS	3.8
1	F	323	VAL	3.8
1	H	351	ASP	3.8
1	C	107	GLY	3.8
1	E	134	TYR	3.7
1	G	429	ALA	3.7
1	B	92	VAL	3.7
1	A	138	PHE	3.7
1	C	256	SER	3.7
1	E	106	PHE	3.7
1	C	201	ALA	3.7
1	A	400	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	344	GLY	3.7
1	A	119	LEU	3.7
1	A	276	ALA	3.7
1	E	389	GLY	3.7
1	C	430	GLU	3.7
1	G	446	LYS	3.7
1	C	8	SER	3.7
1	A	189	GLU	3.7
1	A	226	ALA	3.7
1	G	137	TYR	3.7
1	E	51	PRO	3.7
1	C	309	LEU	3.6
1	H	172	LYS	3.6
1	H	317	ASN	3.6
1	D	218	VAL	3.6
1	F	134	TYR	3.6
1	D	203	LEU	3.6
1	H	14	PHE	3.6
1	C	177	GLU	3.6
1	D	75	CYS	3.6
1	D	22	GLU	3.6
1	E	133	LEU	3.6
1	D	132	ARG	3.6
1	F	95	HIS	3.6
1	F	259	ASP	3.6
1	G	354	VAL	3.6
1	G	236	LYS	3.6
1	G	414	LEU	3.6
1	H	97	PHE	3.5
1	A	419	GLY	3.5
1	B	167	LEU	3.5
1	D	93	TYR	3.5
1	C	299	ALA	3.5
1	F	160	GLY	3.5
1	C	364	LEU	3.5
1	D	400	LEU	3.5
1	A	218	VAL	3.5
1	C	368	PRO	3.5
1	D	376	ASN	3.5
1	B	122	LEU	3.5
1	C	53	PHE	3.5
1	G	396	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	78	ALA	3.5
1	D	33	PRO	3.5
1	D	10	ILE	3.5
1	G	109	TYR	3.5
1	C	77	ARG	3.5
1	H	128	ILE	3.5
1	D	221	GLN	3.5
1	B	198	ARG	3.5
1	D	239	ASP	3.5
1	D	122	LEU	3.5
1	F	366	LYS	3.4
1	D	143	ALA	3.4
1	A	232	PRO	3.4
1	A	146	LEU	3.4
1	B	288	ALA	3.4
1	B	375	ILE	3.4
1	D	306	THR	3.4
1	E	428	ILE	3.4
1	H	374	ILE	3.4
1	H	235	LYS	3.4
1	A	288	ALA	3.4
1	B	44	ALA	3.4
1	D	137	TYR	3.4
1	C	417	THR	3.4
1	G	145	GLY	3.4
1	B	215	TRP	3.4
1	G	418	TYR	3.4
1	A	346	PHE	3.4
1	D	330	ARG	3.4
1	C	116	LYS	3.4
1	G	46	MET	3.4
1	A	217	LEU	3.4
1	G	88	VAL	3.4
1	C	327	ILE	3.4
1	H	236	LYS	3.4
1	F	191	HIS	3.3
1	D	142	GLU	3.3
1	G	431	GLU	3.3
1	G	451	LYS	3.3
1	B	298	LEU	3.3
1	C	260	THR	3.3
1	E	385	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	210	ASN	3.3
1	D	378	GLU	3.3
1	D	335	ALA	3.3
1	E	220	ILE	3.3
1	B	290	GLY	3.3
1	D	424	LEU	3.3
1	E	162	ASP	3.3
1	H	224	ARG	3.3
1	B	229	ILE	3.3
1	G	397	ILE	3.3
1	G	168	PRO	3.3
1	H	133	LEU	3.3
1	A	93	TYR	3.3
1	D	266	TYR	3.3
1	D	406	ILE	3.3
1	G	32	ILE	3.3
1	D	194	ARG	3.3
1	C	425	THR	3.2
1	D	72	THR	3.2
1	E	436	VAL	3.2
1	G	72	THR	3.2
1	D	52	ILE	3.2
1	H	220	ILE	3.2
1	B	355	GLN	3.2
1	E	54	LEU	3.2
1	G	296	ARG	3.2
1	D	135	VAL	3.2
1	E	312	GLY	3.2
1	G	239	ASP	3.2
1	D	412	TRP	3.2
1	G	421	PRO	3.2
1	G	117	MET	3.2
1	B	47	ASN	3.2
1	E	125	GLU	3.2
1	B	258	TYR	3.2
1	D	39	LEU	3.2
1	D	54	LEU	3.2
1	D	115	CYS	3.2
1	F	224	ARG	3.2
1	G	193	ASP	3.2
1	D	101	LEU	3.2
1	H	146	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	67	SER	3.2
1	A	239	ASP	3.2
1	H	33	PRO	3.2
1	C	241	GLY	3.2
1	H	28	SER	3.2
1	H	63	MET	3.2
1	D	441	PHE	3.2
1	A	192	TYR	3.2
1	D	113	LEU	3.2
1	B	43	ASN	3.2
1	A	72	THR	3.2
1	E	259	ASP	3.2
1	H	207	ASP	3.2
1	B	139	GLY	3.2
1	G	213	GLU	3.1
1	C	407	PRO	3.1
1	E	223	ASN	3.1
1	G	111	LYS	3.1
1	A	10	ILE	3.1
1	A	54	LEU	3.1
1	B	138	PHE	3.1
1	C	154	GLN	3.1
1	G	135	VAL	3.1
1	C	434	LEU	3.1
1	F	147	GLU	3.1
1	G	318	THR	3.1
1	C	366	LYS	3.1
1	C	174	ASN	3.1
1	D	82	HIS	3.1
1	F	275	GLY	3.1
1	F	370	MET	3.1
1	D	270	ILE	3.1
1	F	289	ASP	3.0
1	G	447	LEU	3.0
1	A	94	HIS	3.0
1	C	371	VAL	3.0
1	B	262	LEU	3.0
1	A	428	ILE	3.0
1	H	241	GLY	3.0
1	F	94	HIS	3.0
1	G	352	VAL	3.0
1	F	122	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	18	PHE	3.0
1	E	260	THR	3.0
1	C	146	LEU	3.0
1	G	332	VAL	3.0
1	D	340	ASN	3.0
1	G	110	PHE	3.0
1	H	274	THR	3.0
1	A	176	TRP	3.0
1	C	42	ALA	3.0
1	E	341	ALA	3.0
1	E	386	LEU	3.0
1	G	245	GLU	2.9
1	H	125	GLU	2.9
1	H	295	TYR	2.9
1	E	449	GLN	2.9
1	H	285	ALA	2.9
1	H	101	LEU	2.9
1	B	435	VAL	2.9
1	A	35	ASP	2.9
1	D	216	ASN	2.9
1	H	230	LEU	2.9
1	G	368	PRO	2.9
1	B	91	ASP	2.9
1	G	45	GLY	2.9
1	A	96	THR	2.9
1	E	377	GLU	2.9
1	C	141	ASP	2.9
1	D	109	TYR	2.9
1	B	232	PRO	2.9
1	F	84	ASP	2.9
1	D	240	THR	2.9
1	H	424	LEU	2.9
1	H	111	LYS	2.9
1	H	255	MET	2.9
1	G	141	ASP	2.9
1	E	293	MET	2.9
1	F	200	ALA	2.9
1	G	12	GLN	2.8
1	G	312	GLY	2.8
1	H	215	TRP	2.8
1	D	413	LEU	2.8
1	G	304	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	310	ALA	2.8
1	H	301	HIS	2.8
1	C	110	PHE	2.8
1	F	14	PHE	2.8
1	G	386	LEU	2.8
1	A	87	ASP	2.8
1	H	58	ASP	2.8
1	H	9	GLU	2.8
1	H	353	VAL	2.8
1	B	15	ILE	2.8
1	F	207	ASP	2.8
1	H	306	THR	2.8
1	C	216	ASN	2.8
1	E	63	MET	2.8
1	A	287	ASP	2.8
1	C	161	LEU	2.8
1	D	230	LEU	2.8
1	A	250	VAL	2.8
1	C	23	HIS	2.8
1	C	303	ARG	2.8
1	G	188	SER	2.8
1	B	50	LYS	2.8
1	D	262	LEU	2.8
1	C	72	THR	2.8
1	G	123	THR	2.8
1	B	310	ALA	2.8
1	B	282	LYS	2.8
1	G	90	LYS	2.8
1	H	378	GLU	2.8
1	E	423	ASP	2.8
1	F	263	PHE	2.8
1	A	401	GLY	2.8
1	F	29	SER	2.8
1	C	409	ASP	2.8
1	A	39	LEU	2.8
1	F	39	LEU	2.8
1	H	72	THR	2.8
1	D	226	ALA	2.7
1	H	399	SER	2.7
1	D	13	ARG	2.7
1	G	306	THR	2.7
1	H	180	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	104	TRP	2.7
1	C	356	SER	2.7
1	A	300	ASP	2.7
1	B	202	HIS	2.7
1	C	80	GLY	2.7
1	E	156	TRP	2.7
1	G	142	GLU	2.7
1	A	248	VAL	2.7
1	B	191	HIS	2.7
1	F	146	LEU	2.7
1	H	175	PHE	2.7
1	B	104	TRP	2.7
1	G	192	TYR	2.7
1	C	130	ILE	2.7
1	D	229	ILE	2.7
1	F	136	THR	2.7
1	H	394	ASP	2.7
1	E	94	HIS	2.7
1	F	184	CYS	2.7
1	A	291	ILE	2.7
1	C	207	ASP	2.7
1	D	31	THR	2.7
1	F	237	SER	2.7
1	B	81	LYS	2.7
1	D	285	ALA	2.7
1	D	420	PHE	2.7
1	D	371	VAL	2.6
1	G	361	PHE	2.6
1	E	333	ARG	2.6
1	B	261	ASP	2.6
1	H	10	ILE	2.6
1	C	242	MET	2.6
1	D	110	PHE	2.6
1	H	265	PRO	2.6
1	A	450	LEU	2.6
1	C	101	LEU	2.6
1	D	138	PHE	2.6
1	H	197	GLY	2.6
1	B	327	ILE	2.6
1	B	406	ILE	2.6
1	C	71	ASN	2.6
1	F	437	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	80	GLY	2.6
1	E	249	SER	2.6
1	H	145	GLY	2.6
1	H	156	TRP	2.6
1	H	305	ILE	2.6
1	C	143	ALA	2.6
1	C	73	GLN	2.6
1	G	427	LEU	2.6
1	E	346	PHE	2.6
1	H	313	GLY	2.6
1	A	315	PRO	2.6
1	F	190	ILE	2.6
1	A	380	VAL	2.6
1	B	149	ASP	2.6
1	C	233	LEU	2.6
1	C	298	LEU	2.5
1	C	281	GLY	2.5
1	H	102	GLY	2.5
1	D	83	ASN	2.5
1	G	406	ILE	2.5
1	A	422	VAL	2.5
1	G	393	LEU	2.5
1	G	424	LEU	2.5
1	H	434	LEU	2.5
1	E	445	ARG	2.5
1	H	126	PHE	2.5
1	C	317	ASN	2.5
1	A	24	THR	2.5
1	H	56	THR	2.5
1	E	222	TYR	2.5
1	F	81	LYS	2.5
1	F	246	ARG	2.5
1	A	216	ASN	2.5
1	E	390	ARG	2.5
1	H	139	GLY	2.5
1	D	357	LEU	2.5
1	D	53	PHE	2.5
1	D	81	LYS	2.5
1	E	33	PRO	2.5
1	E	405	THR	2.5
1	H	433	GLY	2.5
1	B	161	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	133	LEU	2.5
1	H	217	LEU	2.5
1	D	177	GLU	2.5
1	G	18	PHE	2.5
1	E	231	LYS	2.5
1	H	170	ASN	2.5
1	B	367	ASP	2.5
1	B	368	PRO	2.5
1	E	299	ALA	2.5
1	G	228	GLY	2.5
1	D	327	ILE	2.5
1	A	121	LEU	2.5
1	F	383	LEU	2.5
1	A	441	PHE	2.5
1	F	110	PHE	2.5
1	D	24	THR	2.5
1	G	305	ILE	2.5
1	B	447	LEU	2.5
1	C	50	LYS	2.5
1	C	263	PHE	2.5
1	D	185	GLY	2.4
1	H	142	GLU	2.4
1	F	285	ALA	2.4
1	A	214	ILE	2.4
1	C	215	TRP	2.4
1	D	422	VAL	2.4
1	A	222	TYR	2.4
1	A	12	GLN	2.4
1	G	80	GLY	2.4
1	G	265	PRO	2.4
1	G	407	PRO	2.4
1	H	315	PRO	2.4
1	C	11	ARG	2.4
1	A	361	PHE	2.4
1	C	126	PHE	2.4
1	A	127	GLY	2.4
1	E	178	MET	2.4
1	B	234	PRO	2.4
1	C	176	TRP	2.4
1	D	219	PHE	2.4
1	E	111	LYS	2.4
1	B	145	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	178	MET	2.4
1	H	209	PRO	2.4
1	B	294	ALA	2.4
1	D	38	THR	2.4
1	F	32	ILE	2.4
1	F	396	LYS	2.4
1	F	406	ILE	2.4
1	H	76	ILE	2.4
1	C	307	VAL	2.4
1	F	297	VAL	2.4
1	A	240	THR	2.4
1	D	148	ALA	2.4
1	E	285	ALA	2.4
1	F	298	LEU	2.4
1	D	397	ILE	2.4
1	A	411	ALA	2.4
1	C	240	THR	2.4
1	E	403	SER	2.4
1	E	155	ILE	2.4
1	C	169	GLY	2.4
1	H	273	GLY	2.4
1	H	49	PHE	2.4
1	C	111	LYS	2.4
1	B	25	TYR	2.4
1	A	206	GLN	2.4
1	B	85	LEU	2.4
1	G	47	ASN	2.4
1	C	49	PHE	2.4
1	H	303	ARG	2.4
1	A	63	MET	2.3
1	A	129	PRO	2.3
1	A	439	ASP	2.3
1	E	36	ASP	2.3
1	E	294	ALA	2.3
1	B	231	LYS	2.3
1	H	99	GLU	2.3
1	G	48	GLN	2.3
1	H	37	PRO	2.3
1	H	322	TYR	2.3
1	B	274	THR	2.3
1	C	56	THR	2.3
1	C	114	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	247	LEU	2.3
1	F	42	ALA	2.3
1	F	434	LEU	2.3
1	G	253	ASN	2.3
1	D	41	PHE	2.3
1	B	124	GLN	2.3
1	F	176	TRP	2.3
1	G	85	LEU	2.3
1	G	329	ARG	2.3
1	A	221	GLN	2.3
1	C	384	LYS	2.3
1	C	108	ASP	2.3
1	C	351	ASP	2.3
1	H	337	GLU	2.3
1	A	212	LEU	2.3
1	E	298	LEU	2.3
1	G	358	GLY	2.3
1	D	116	LYS	2.3
1	G	49	PHE	2.3
1	D	99	GLU	2.3
1	G	203	LEU	2.3
1	G	370	MET	2.3
1	H	122	LEU	2.3
1	H	242	MET	2.3
1	C	404	LYS	2.3
1	F	49	PHE	2.3
1	D	163	ASP	2.3
1	A	389	GLY	2.3
1	F	234	PRO	2.3
1	E	375	ILE	2.3
1	F	345	PHE	2.3
1	F	422	VAL	2.3
1	C	230	LEU	2.3
1	E	237	SER	2.3
1	D	118	ALA	2.3
1	C	181	THR	2.3
1	H	6	THR	2.3
1	C	68	ARG	2.3
1	C	76	ILE	2.3
1	G	172	LYS	2.3
1	E	444	GLU	2.2
1	F	286	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	69	ALA	2.2
1	F	109	TYR	2.2
1	B	170	ASN	2.2
1	G	234	PRO	2.2
1	G	249	SER	2.2
1	H	188	SER	2.2
1	E	335	ALA	2.2
1	F	132	ARG	2.2
1	B	18	PHE	2.2
1	E	190	ILE	2.2
1	H	140	GLY	2.2
1	B	27	HIS	2.2
1	E	55	ASN	2.2
1	E	34	LEU	2.2
1	H	68	ARG	2.2
1	F	258	TYR	2.2
1	G	322	TYR	2.2
1	F	353	VAL	2.2
1	F	371	VAL	2.2
1	H	214	ILE	2.2
1	A	170	ASN	2.2
1	G	23	HIS	2.2
1	H	314	ARG	2.2
1	C	24	THR	2.2
1	A	196	GLY	2.2
1	A	14	PHE	2.2
1	B	317	ASN	2.2
1	B	445	ARG	2.2
1	H	395	ARG	2.2
1	A	19	LYS	2.2
1	E	425	THR	2.2
1	C	361	PHE	2.2
1	F	262	LEU	2.2
1	H	104	TRP	2.2
1	B	140	GLY	2.2
1	H	261	ASP	2.2
1	F	18	PHE	2.2
1	C	192	TYR	2.2
1	A	55	ASN	2.2
1	B	237	SER	2.2
1	G	350	VAL	2.2
1	B	217	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLY	2.2
1	D	223	ASN	2.1
1	F	334	TYR	2.1
1	G	404	LYS	2.1
1	B	52	ILE	2.1
1	B	270	ILE	2.1
1	G	190	ILE	2.1
1	H	211	VAL	2.1
1	G	364	LEU	2.1
1	H	393	LEU	2.1
1	E	290	GLY	2.1
1	A	448	ALA	2.1
1	G	325	ARG	2.1
1	D	154	GLN	2.1
1	D	59	PRO	2.1
1	F	31	THR	2.1
1	F	156	TRP	2.1
1	F	215	TRP	2.1
1	G	338	LYS	2.1
1	E	75	CYS	2.1
1	B	94	HIS	2.1
1	H	159	LEU	2.1
1	C	365	LYS	2.1
1	C	226	ALA	2.1
1	D	200	ALA	2.1
1	G	242	MET	2.1
1	A	175	PHE	2.1
1	A	128	ILE	2.1
1	B	116	LYS	2.1
1	C	393	LEU	2.1
1	D	328	LEU	2.1
1	D	428	ILE	2.1
1	E	322	TYR	2.1
1	F	236	LYS	2.1
1	G	261	ASP	2.1
1	H	297	VAL	2.1
1	H	234	PRO	2.1
1	F	335	ALA	2.1
1	H	201	ALA	2.1
1	G	6	THR	2.1
1	B	150	LEU	2.1
1	C	291	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	211	VAL	2.1
1	D	386	LEU	2.1
1	B	315	PRO	2.1
1	C	61	HIS	2.1
1	F	244	LEU	2.1
1	D	170	ASN	2.1
1	C	20	ARG	2.1
1	E	277	ARG	2.1
1	E	296	ARG	2.1
1	F	53	PHE	2.1
1	H	194	ARG	2.1
1	B	58	ASP	2.1
1	C	87	ASP	2.1
1	A	113	LEU	2.1
1	B	247	LEU	2.1
1	B	323	VAL	2.1
1	F	168	PRO	2.1
1	H	355	GLN	2.1
1	H	404	LYS	2.1
1	A	304	THR	2.1
1	C	253	ASN	2.1
1	E	275	GLY	2.1
1	D	212	LEU	2.1
1	B	225	GLU	2.1
1	H	67	SER	2.1
1	E	267	PHE	2.1
1	H	185	GLY	2.1
1	A	323	VAL	2.0
1	H	192	TYR	2.0
1	B	311	ASP	2.0
1	C	188	SER	2.0
1	G	17	PHE	2.0
1	H	98	PHE	2.0
1	H	272	LYS	2.0
1	C	85	LEU	2.0
1	F	34	LEU	2.0
1	G	186	PRO	2.0
1	G	204	VAL	2.0
1	D	222	TYR	2.0
1	H	216	ASN	2.0
1	H	411	ALA	2.0
1	B	182	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	387	SER	2.0
1	H	281	GLY	2.0
1	G	157	GLN	2.0
1	H	449	GLN	2.0
1	B	434	LEU	2.0
1	D	85	LEU	2.0
1	E	427	LEU	2.0
1	B	186	PRO	2.0
1	G	422	VAL	2.0
1	F	52	ILE	2.0
1	F	270	ILE	2.0
1	A	432	LYS	2.0
1	C	79	GLY	2.0
1	B	277	ARG	2.0
1	G	40	LEU	2.0
1	F	88	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	A5A	E	500	28/28	0.90	0.24	-0.18	20,24,46,63	0
2	A5A	D	500	28/28	0.89	0.29	-0.47	41,52,59,62	0
2	A5A	G	500	28/28	0.90	0.23	-0.58	22,53,68,75	0
2	A5A	B	500	28/28	0.91	0.23	-0.63	24,36,49,53	0
2	A5A	F	500	28/28	0.91	0.22	-0.86	26,32,35,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	A5A	A	500	28/28	0.87	0.21	-0.87	28,34,43,47	0
2	A5A	C	500	28/28	0.89	0.20	-1.12	43,52,63,65	0
2	A5A	H	500	28/28	0.88	0.21	-1.26	35,48,53,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.