



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:39 am GMT

PDB ID : 5J6R
Title : Crystal structure of Human Papillomavirus Type 59 L1 pentamer
Authors : Li, Z.H.; Yan, X.D.; Yu, H.; Gu, Y.; Li, S.W.
Deposited on : 2016-04-05
Resolution : 4.01 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

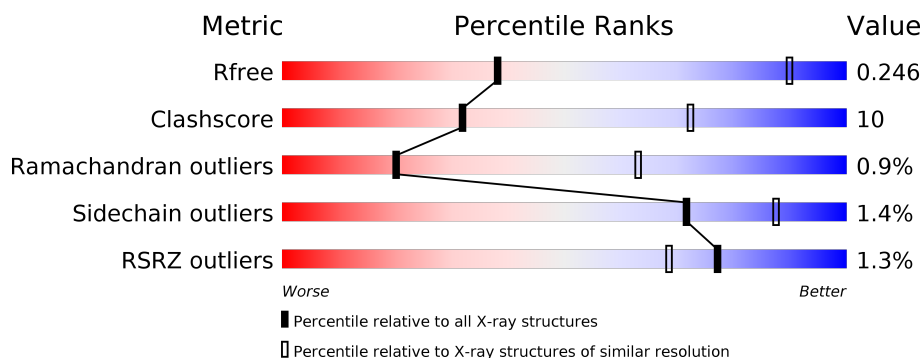
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.01 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}	100719	1089 (4.42-3.60)
Clashscore	112137	1189 (4.44-3.60)
Ramachandran outliers	110173	1140 (4.42-3.60)
Sidechain outliers	110143	1127 (4.42-3.60)
RSRZ outliers	101464	1100 (4.42-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	500	<div> <div style="width: 63%;"></div> <div style="width: 21%;"></div> <div style="width: 16%;"></div> </div> <div>63% 21% 16%</div>
1	B	500	<div> <div style="width: 61%;"></div> <div style="width: 21%;"></div> <div style="width: 17%;"></div> </div> <div>61% 21% 17%</div>
1	C	500	<div> <div style="width: 62%;"></div> <div style="width: 21%;"></div> <div style="width: 16%;"></div> </div> <div>62% 21% 16%</div>
1	D	500	<div> <div style="width: 63%;"></div> <div style="width: 20%;"></div> <div style="width: 16%;"></div> </div> <div>63% 20% 16%</div>
1	E	500	<div> <div style="width: 63%;"></div> <div style="width: 20%;"></div> <div style="width: 16%;"></div> </div> <div>63% 20% 16%</div>
1	F	500	<div> <div style="width: 62%;"></div> <div style="width: 22%;"></div> <div style="width: 16%;"></div> </div> <div>62% 22% 16%</div>

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Mol	Chain	Length	Quality of chain
1	G	500	<div><div><div>%</div><div><div></div><div>62%</div><div>21%</div><div>•</div><div>16%</div></div></div></div>
1	H	500	<div><div><div>%</div><div><div></div><div>61%</div><div>21%</div><div>•</div><div>17%</div></div></div></div>
1	I	500	<div><div><div>%</div><div><div></div><div>63%</div><div>20%</div><div>•</div><div>16%</div></div></div></div>
1	J	500	<div><div><div>%</div><div><div></div><div>63%</div><div>20%</div><div>•</div><div>16%</div></div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33270 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	B	416	Total	C	N	O	S	0	0	0
			3305	2101	556	631	17			
1	C	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	D	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	E	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	F	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	G	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	H	414	Total	C	N	O	S	0	0	0
			3293	2094	554	628	17			
1	I	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	J	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP Q81971
A	175	SER	CYS	engineered mutation	UNP Q81971
B	9	MET	-	initiating methionine	UNP Q81971
B	175	SER	CYS	engineered mutation	UNP Q81971
C	9	MET	-	initiating methionine	UNP Q81971
C	175	SER	CYS	engineered mutation	UNP Q81971
D	9	MET	-	initiating methionine	UNP Q81971
D	175	SER	CYS	engineered mutation	UNP Q81971
E	9	MET	-	initiating methionine	UNP Q81971

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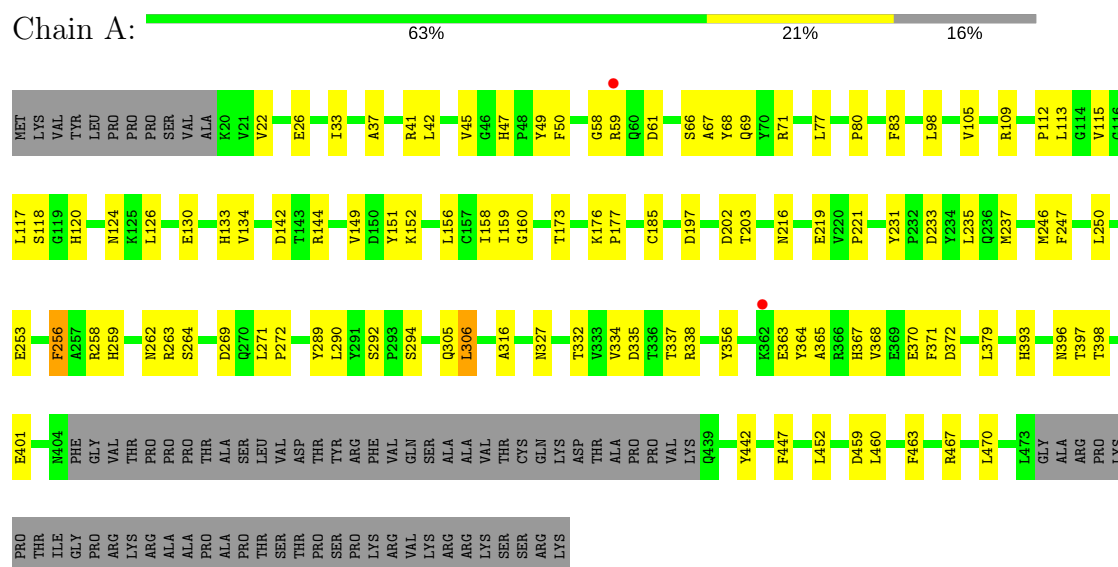
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Chain	Residue	Modelled	Actual	Comment	Reference
E	175	SER	CYS	engineered mutation	UNP Q81971
F	9	MET	-	initiating methionine	UNP Q81971
F	175	SER	CYS	engineered mutation	UNP Q81971
G	9	MET	-	initiating methionine	UNP Q81971
G	175	SER	CYS	engineered mutation	UNP Q81971
H	9	MET	-	initiating methionine	UNP Q81971
H	175	SER	CYS	engineered mutation	UNP Q81971
I	9	MET	-	initiating methionine	UNP Q81971
I	175	SER	CYS	engineered mutation	UNP Q81971
J	9	MET	-	initiating methionine	UNP Q81971
J	175	SER	CYS	engineered mutation	UNP Q81971

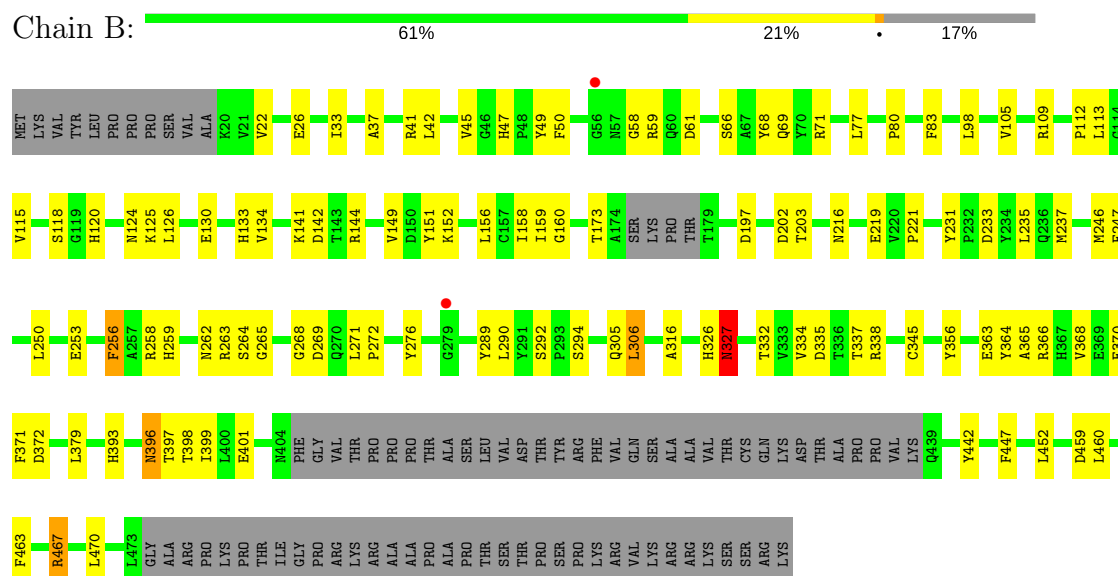
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Major capsid protein L1

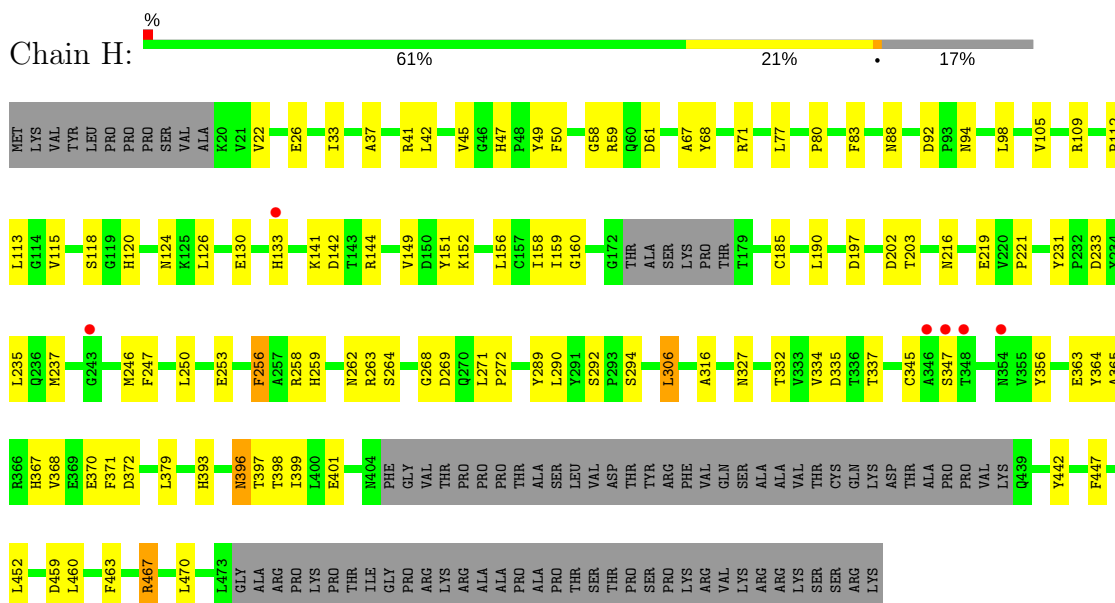


• Molecule 1: Major capsid protein L1

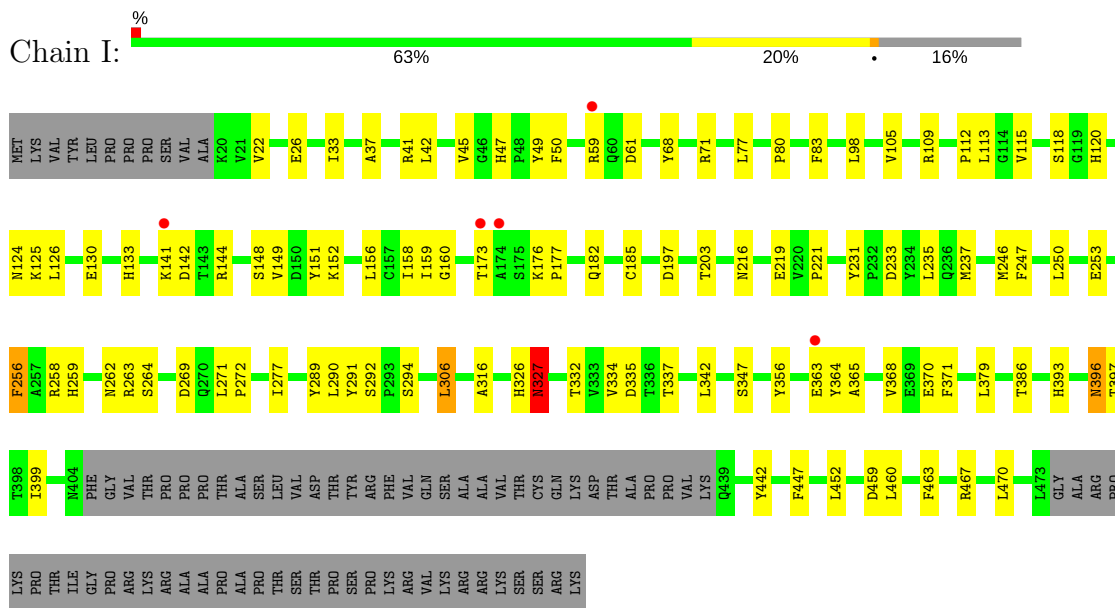


Chain E:

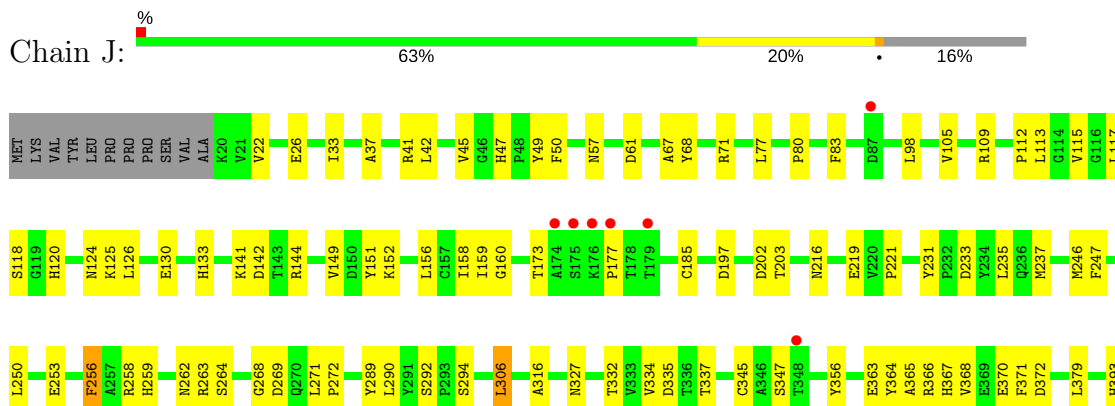
Amino Acid	Frequency (%)
MET	2%
LYS	63%
VAL	63%
LEU	63%
PRO	63%
PRO	63%
PRO	63%
SER	63%
VAL	63%
ALA	63%
K20	20%
V21	20%
V22	20%
E26	20%
I33	20%
A37	20%
R41	20%
L42	20%
V45	20%
G46	20%
H47	20%
F48	20%
Y49	20%
F50	20%
G56	20%
N57	20%
G58	20%
R59	20%
R60	20%
D61	20%
Y68	20%
R71	20%
L77	20%
P80	20%
F83	20%
R88	20%
L98	20%
V105	20%
R109	20%
P112	20%
L113	20%
G114	20%
V115	20%
S118	16%
G119	16%
H120	16%
N124	16%
K125	16%
L126	16%
E130	16%
H133	16%
K141	16%
D142	16%
T143	16%
R144	16%
S148	16%
V149	16%
D150	16%
Y151	16%
K152	16%
L156	16%
C157	16%
I158	16%
I159	16%
G160	16%
T173	16%
A174	16%
S175	16%
K176	16%
P177	16%
C185	16%
D197	16%
D202	16%
T203	16%
N216	16%
K217	16%
S218	16%
E219	16%
V220	16%
P221	16%
Y231	16%
P232	16%
D233	16%
Y234	16%
L235	16%
Q236	16%
M237	16%
M246	16%
T247	16%



- Molecule 1: Major capsid protein L1



- Molecule 1: Major capsid protein L1



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.24Å 161.74Å 154.73Å 90.00° 110.34° 90.00°	Depositor
Resolution (Å)	49.70 – 4.01 49.70 – 4.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.70-4.01) 99.3 (49.70-4.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.243 , 0.267 0.223 , 0.246	Depositor DCC
R_{free} test set	2231 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	1.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	33270	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	0/3421	0.43	0/4656
1	B	0.48	5/3390 (0.1%)	0.62	3/4612 (0.1%)
1	C	0.26	1/3421 (0.0%)	0.43	0/4656
1	D	0.29	0/3421	0.64	5/4656 (0.1%)
1	E	0.30	2/3421 (0.1%)	0.43	0/4656
1	F	0.27	1/3421 (0.0%)	0.45	1/4656 (0.0%)
1	G	0.23	0/3421	0.42	0/4656
1	H	0.23	0/3378	0.42	1/4595 (0.0%)
1	I	0.27	1/3421 (0.0%)	0.43	0/4656
1	J	0.23	0/3421	0.42	0/4656
All	All	0.29	10/34136 (0.0%)	0.48	10/46455 (0.0%)

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	D	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	TYR	CG-CD2	-12.48	1.23	1.39
1	B	276	TYR	CG-CD1	-12.19	1.23	1.39
1	B	276	TYR	CE1-CZ	-10.87	1.24	1.38
1	B	276	TYR	CE2-CZ	-9.84	1.25	1.38
1	E	327	ASN	CG-OD1	-7.29	1.07	1.24
1	F	306	LEU	CB-CG	-5.64	1.36	1.52
1	E	327	ASN	CG-ND2	-5.35	1.19	1.32
1	C	327	ASN	CG-ND2	5.31	1.46	1.32
1	I	327	ASN	CG-ND2	5.30	1.46	1.32
1	B	327	ASN	CG-ND2	5.23	1.46	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	ARG	NE-CZ-NH1	-19.69	110.46	120.30
1	D	467	ARG	NE-CZ-NH1	-19.51	110.54	120.30
1	B	467	ARG	NE-CZ-NH2	19.44	130.02	120.30
1	D	467	ARG	NE-CZ-NH2	19.32	129.96	120.30
1	D	467	ARG	CD-NE-CZ	9.71	137.19	123.60
1	B	467	ARG	CD-NE-CZ	9.63	137.08	123.60
1	F	306	LEU	CB-CG-CD2	6.23	121.59	111.00
1	D	461	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	D	377	PHE	CB-CG-CD1	-5.15	117.19	120.80
1	H	467	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	461	ASP	Sidechain

5.2 Too-close contacts [i](#)

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	3334	0	3234	75	0
1	B	3305	0	3201	82	0
1	C	3334	0	3234	84	0
1	D	3334	0	3234	76	1
1	E	3334	0	3234	77	0
1	F	3334	0	3234	81	2
1	G	3334	0	3234	78	1
1	H	3293	0	3189	81	1
1	I	3334	0	3234	81	2
1	J	3334	0	3234	78	1
All	All	33270	0	32262	662	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 10.

All (662) 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:C:41:ARG:NH2	1:H:233:ASP:OD2	2.18	0.76
1:B:290:LEU:HD22	1:D:363:GLU:HB3	1.68	0.74
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.72	0.72
1:F:233:ASP:OD2	1:J:41:ARG:NH2	2.23	0.72
1:J:126:LEU:HB3	1:J:262:ASN:HB3	1.72	0.72
1:I:126:LEU:HB3	1:I:262:ASN:HB3	1.72	0.72
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.72	0.72
1:C:356:TYR:HE2	1:H:142:ASP:HB3	1.55	0.71
1:H:237:MET:HB3	1:H:246:MET:HG2	1.72	0.71
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.72	0.71
1:I:237:MET:HB3	1:I:246:MET:HG2	1.72	0.71
1:F:126:LEU:HB3	1:F:262:ASN:HB3	1.72	0.71
1:E:290:LEU:HD22	1:F:363:GLU:HB3	1.72	0.71
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.72	0.71
1:E:233:ASP:OD2	1:F:41:ARG:NH2	2.23	0.71
1:G:237:MET:HB3	1:G:246:MET:HG2	1.72	0.71
1:D:237:MET:HB3	1:D:246:MET:HG2	1.73	0.71
1:I:47:HIS:HD2	1:I:50:PHE:H	1.39	0.71
1:H:126:LEU:HB3	1:H:262:ASN:HB3	1.72	0.71
1:C:47:HIS:HD2	1:C:50:PHE:H	1.39	0.70
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.73	0.70
1:E:237:MET:HB3	1:E:246:MET:HG2	1.73	0.70
1:F:47:HIS:HD2	1:F:50:PHE:H	1.38	0.70
1:J:47:HIS:HD2	1:J:50:PHE:H	1.38	0.70
1:E:47:HIS:HD2	1:E:50:PHE:H	1.39	0.70
1:B:237:MET:HB3	1:B:246:MET:HG2	1.72	0.70
1:C:237:MET:HB3	1:C:246:MET:HG2	1.73	0.70
1:F:237:MET:HB3	1:F:246:MET:HG2	1.72	0.70
1:E:41:ARG:NH2	1:I:233:ASP:OD2	2.24	0.70
1:G:126:LEU:HB3	1:G:262:ASN:HB3	1.72	0.70
1:H:47:HIS:HD2	1:H:50:PHE:H	1.39	0.70
1:H:142:ASP:HB2	1:H:144:ARG:HG2	1.73	0.70
1:I:142:ASP:HB2	1:I:144:ARG:HG2	1.74	0.70
1:D:142:ASP:HB2	1:D:144:ARG:HG2	1.74	0.69
1:A:237:MET:HB3	1:A:246:MET:HG2	1.72	0.69
1:B:47:HIS:HD2	1:B:50:PHE:H	1.38	0.69
1:C:363:GLU:HB3	1:H:290:LEU:HD22	1.73	0.69
1:G:142:ASP:HB2	1:G:144:ARG:HG2	1.74	0.69
1:J:237:MET:HB3	1:J:246:MET:HG2	1.72	0.69
1:J:142:ASP:HB2	1:J:144:ARG:HG2	1.74	0.69
1:A:47:HIS:HD2	1:A:50:PHE:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:HB2	1:A:144:ARG:HG2	1.74	0.69
1:D:47:HIS:HD2	1:D:50:PHE:H	1.39	0.69
1:C:142:ASP:HB2	1:C:144:ARG:HG2	1.74	0.69
1:G:47:HIS:HD2	1:G:50:PHE:H	1.38	0.68
1:A:363:GLU:HB3	1:C:290:LEU:HD22	1.75	0.68
1:G:363:GLU:HB3	1:J:290:LEU:HD22	1.75	0.68
1:E:142:ASP:HB2	1:E:144:ARG:HG2	1.74	0.68
1:F:142:ASP:HB2	1:F:144:ARG:HG2	1.74	0.68
1:B:142:ASP:HB2	1:B:144:ARG:HG2	1.74	0.67
1:B:80:PRO:HD3	1:B:327:ASN:OD1	1.95	0.67
1:B:233:ASP:OD2	1:D:41:ARG:NH2	2.28	0.67
1:D:247:PHE:HB2	1:D:316:ALA:HB1	1.76	0.67
1:D:71:ARG:NH2	1:D:197:ASP:OD1	2.28	0.66
1:D:233:ASP:OD2	1:H:41:ARG:NH2	2.29	0.66
1:G:41:ARG:NH2	1:J:233:ASP:OD2	2.28	0.66
1:I:80:PRO:HD3	1:I:327:ASN:OD1	1.95	0.66
1:H:247:PHE:HB2	1:H:316:ALA:HB1	1.78	0.66
1:A:71:ARG:NH2	1:A:197:ASP:OD1	2.29	0.66
1:A:233:ASP:OD2	1:B:41:ARG:NH2	2.28	0.66
1:E:247:PHE:HB2	1:E:316:ALA:HB1	1.78	0.66
1:F:247:PHE:HB2	1:F:316:ALA:HB1	1.78	0.66
1:C:356:TYR:CE2	1:H:142:ASP:HB3	2.31	0.66
1:J:247:PHE:HB2	1:J:316:ALA:HB1	1.78	0.66
1:J:71:ARG:NH2	1:J:197:ASP:OD1	2.29	0.66
1:E:71:ARG:NH2	1:E:197:ASP:OD1	2.29	0.66
1:G:71:ARG:NH2	1:G:197:ASP:OD1	2.29	0.66
1:C:80:PRO:HD3	1:C:327:ASN:OD1	1.95	0.66
1:I:247:PHE:HB2	1:I:316:ALA:HB1	1.78	0.66
1:G:247:PHE:HB2	1:G:316:ALA:HB1	1.78	0.65
1:A:142:ASP:HB3	1:B:356:TYR:HE2	1.60	0.65
1:C:247:PHE:HB2	1:C:316:ALA:HB1	1.78	0.65
1:A:247:PHE:HB2	1:A:316:ALA:HB1	1.78	0.65
1:B:71:ARG:NH2	1:B:197:ASP:OD1	2.29	0.65
1:I:71:ARG:NH2	1:I:197:ASP:OD1	2.29	0.65
1:B:247:PHE:HB2	1:B:316:ALA:HB1	1.78	0.65
1:E:356:TYR:HE2	1:I:142:ASP:HB3	1.61	0.65
1:G:356:TYR:HE2	1:J:142:ASP:HB3	1.61	0.65
1:A:41:ARG:NH2	1:C:233:ASP:OD2	2.31	0.64
1:H:71:ARG:NH2	1:H:197:ASP:OD1	2.29	0.64
1:F:71:ARG:NH2	1:F:197:ASP:OD1	2.31	0.63
1:C:71:ARG:NH2	1:C:197:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:HD22	1:H:363:GLU:HB3	1.80	0.63
1:F:290:LEU:HD22	1:J:363:GLU:HB3	1.80	0.62
1:A:356:TYR:HE2	1:C:142:ASP:HB3	1.63	0.62
1:E:363:GLU:HB3	1:I:290:LEU:HD22	1.82	0.62
1:G:253:GLU:HG3	1:I:113:LEU:HD12	1.82	0.61
1:B:142:ASP:HB3	1:D:356:TYR:HE2	1.65	0.61
1:A:290:LEU:HD22	1:B:363:GLU:HB3	1.81	0.61
1:C:326:HIS:C	1:C:327:ASN:HD22	2.04	0.60
1:B:120:HIS:HB2	1:B:221:PRO:HA	1.84	0.60
1:F:253:GLU:HG3	1:J:113:LEU:HD12	1.83	0.60
1:I:120:HIS:HB2	1:I:221:PRO:HA	1.84	0.60
1:G:120:HIS:HB2	1:G:221:PRO:HA	1.83	0.60
1:I:326:HIS:C	1:I:327:ASN:HD22	2.05	0.60
1:D:120:HIS:HB2	1:D:221:PRO:HA	1.84	0.60
1:B:326:HIS:C	1:B:327:ASN:HD22	2.04	0.60
1:A:120:HIS:HB2	1:A:221:PRO:HA	1.84	0.59
1:E:142:ASP:HB3	1:F:356:TYR:HE2	1.66	0.59
1:G:290:LEU:HD22	1:I:363:GLU:HB3	1.84	0.59
1:G:356:TYR:CE2	1:J:142:ASP:HB3	2.37	0.59
1:C:120:HIS:HB2	1:C:221:PRO:HA	1.84	0.59
1:E:120:HIS:HB2	1:E:221:PRO:HA	1.84	0.59
1:J:45:VAL:HG12	1:J:368:VAL:HG22	1.85	0.59
1:C:45:VAL:HG12	1:C:368:VAL:HG22	1.85	0.59
1:G:45:VAL:HG12	1:G:368:VAL:HG22	1.85	0.59
1:H:120:HIS:HB2	1:H:221:PRO:HA	1.84	0.59
1:A:45:VAL:HG12	1:A:368:VAL:HG22	1.85	0.59
1:F:142:ASP:HB3	1:J:356:TYR:HE2	1.67	0.59
1:I:45:VAL:HG12	1:I:368:VAL:HG22	1.85	0.59
1:B:45:VAL:HG12	1:B:368:VAL:HG22	1.85	0.59
1:F:45:VAL:HG12	1:F:368:VAL:HG22	1.85	0.59
1:G:233:ASP:OD2	1:I:41:ARG:NH2	2.36	0.59
1:H:45:VAL:HG12	1:H:368:VAL:HG22	1.85	0.59
1:J:120:HIS:HB2	1:J:221:PRO:HA	1.84	0.59
1:F:120:HIS:HB2	1:F:221:PRO:HA	1.84	0.58
1:E:256:PHE:HA	1:F:115:VAL:HG21	1.85	0.58
1:A:142:ASP:HB3	1:B:356:TYR:CE2	2.38	0.58
1:A:113:LEU:HD12	1:C:253:GLU:HG3	1.86	0.58
1:B:142:ASP:HB3	1:D:356:TYR:CE2	2.39	0.58
1:E:45:VAL:HG12	1:E:368:VAL:HG22	1.85	0.57
1:D:45:VAL:HG12	1:D:368:VAL:HG22	1.85	0.57
1:C:115:VAL:HG21	1:H:256:PHE:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:TYR:CE2	1:C:142:ASP:HB3	2.39	0.57
1:E:356:TYR:CE2	1:I:142:ASP:HB3	2.40	0.57
1:I:49:TYR:HE1	1:I:118:SER:HA	1.70	0.57
1:H:49:TYR:HE1	1:H:118:SER:HA	1.70	0.57
1:C:49:TYR:HE1	1:C:118:SER:HA	1.70	0.56
1:D:142:ASP:HB3	1:H:356:TYR:HE2	1.70	0.56
1:E:49:TYR:HE1	1:E:118:SER:HA	1.70	0.56
1:B:256:PHE:HA	1:D:115:VAL:HG21	1.87	0.56
1:D:49:TYR:HE1	1:D:118:SER:HA	1.70	0.56
1:A:115:VAL:HG21	1:C:256:PHE:HA	1.87	0.56
1:D:253:GLU:HG3	1:H:113:LEU:HD12	1.87	0.56
1:B:49:TYR:HE1	1:B:118:SER:HA	1.70	0.56
1:G:142:ASP:HB3	1:I:356:TYR:HE2	1.71	0.56
1:H:109:ARG:NH1	1:H:370:GLU:O	2.39	0.56
1:J:49:TYR:HE1	1:J:118:SER:HA	1.70	0.56
1:A:49:TYR:HE1	1:A:118:SER:HA	1.70	0.55
1:D:109:ARG:NH1	1:D:370:GLU:O	2.39	0.55
1:F:256:PHE:HA	1:J:115:VAL:HG21	1.88	0.55
1:C:109:ARG:NH1	1:C:370:GLU:O	2.39	0.55
1:F:49:TYR:HE1	1:F:118:SER:HA	1.71	0.55
1:G:109:ARG:NH1	1:G:370:GLU:O	2.40	0.55
1:B:109:ARG:NH1	1:B:370:GLU:O	2.39	0.55
1:E:109:ARG:NH1	1:E:370:GLU:O	2.40	0.55
1:J:109:ARG:NH1	1:J:370:GLU:O	2.40	0.55
1:G:49:TYR:HE1	1:G:118:SER:HA	1.70	0.55
1:A:109:ARG:NH1	1:A:370:GLU:O	2.40	0.55
1:F:109:ARG:NH1	1:F:370:GLU:O	2.39	0.54
1:E:142:ASP:HB3	1:F:356:TYR:CE2	2.42	0.54
1:G:115:VAL:HG21	1:J:256:PHE:HA	1.90	0.54
1:I:109:ARG:NH1	1:I:370:GLU:O	2.40	0.54
1:I:142:ASP:N	1:I:142:ASP:OD1	2.36	0.54
1:F:231:TYR:CD1	1:J:112:PRO:HB3	2.43	0.54
1:J:269:ASP:O	1:J:289:TYR:OH	2.21	0.54
1:E:345:CYS:SG	1:I:216:ASN:HB2	2.47	0.54
1:G:231:TYR:CD1	1:I:112:PRO:HB3	2.43	0.54
1:C:142:ASP:OD1	1:C:142:ASP:N	2.36	0.54
1:I:263:ARG:HB2	1:I:290:LEU:HB3	1.91	0.53
1:E:152:LYS:HE3	1:E:253:GLU:HB2	1.91	0.53
1:E:263:ARG:HB2	1:E:290:LEU:HB3	1.92	0.53
1:C:61:ASP:N	1:C:61:ASP:OD1	2.43	0.52
1:I:459:ASP:N	1:I:459:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:152:LYS:NZ	1:J:202:ASP:OD2	2.37	0.52
1:B:263:ARG:HB2	1:B:290:LEU:HB3	1.91	0.52
1:B:459:ASP:N	1:B:459:ASP:OD1	2.42	0.52
1:C:345:CYS:SG	1:H:216:ASN:HB2	2.49	0.52
1:F:142:ASP:OD1	1:F:142:ASP:N	2.36	0.52
1:F:61:ASP:N	1:F:61:ASP:OD1	2.43	0.52
1:J:263:ARG:HB2	1:J:290:LEU:HB3	1.91	0.52
1:B:61:ASP:OD1	1:B:61:ASP:N	2.42	0.52
1:J:459:ASP:N	1:J:459:ASP:OD1	2.42	0.52
1:A:109:ARG:NE	1:A:335:ASP:OD2	2.38	0.52
1:G:263:ARG:HB2	1:G:290:LEU:HB3	1.91	0.52
1:G:61:ASP:N	1:G:61:ASP:OD1	2.43	0.52
1:I:61:ASP:N	1:I:61:ASP:OD1	2.43	0.52
1:A:61:ASP:OD1	1:A:61:ASP:N	2.42	0.52
1:C:263:ARG:HB2	1:C:290:LEU:HB3	1.91	0.52
1:H:61:ASP:N	1:H:61:ASP:OD1	2.43	0.52
1:C:80:PRO:HA	1:C:83:PHE:HB2	1.92	0.52
1:D:61:ASP:OD1	1:D:61:ASP:N	2.43	0.52
1:G:459:ASP:OD1	1:G:459:ASP:N	2.42	0.52
1:G:80:PRO:HA	1:G:83:PHE:HB2	1.92	0.52
1:A:80:PRO:HA	1:A:83:PHE:HB2	1.92	0.52
1:E:77:LEU:HB2	1:E:327:ASN:HB3	1.92	0.52
1:E:459:ASP:N	1:E:459:ASP:OD1	2.43	0.52
1:J:61:ASP:OD1	1:J:61:ASP:N	2.43	0.52
1:I:80:PRO:HA	1:I:83:PHE:HB2	1.92	0.52
1:B:37:ALA:HB1	1:B:452:LEU:HD13	1.92	0.51
1:D:256:PHE:HA	1:H:115:VAL:HG21	1.90	0.51
1:E:61:ASP:N	1:E:61:ASP:OD1	2.42	0.51
1:A:152:LYS:HE3	1:A:253:GLU:HB2	1.92	0.51
1:B:80:PRO:HA	1:B:83:PHE:HB2	1.92	0.51
1:C:152:LYS:NZ	1:C:202:ASP:OD2	2.37	0.51
1:D:80:PRO:HA	1:D:83:PHE:HB2	1.92	0.51
1:E:80:PRO:HA	1:E:83:PHE:HB2	1.93	0.51
1:J:142:ASP:OD1	1:J:142:ASP:N	2.36	0.51
1:J:152:LYS:HE3	1:J:253:GLU:HB2	1.92	0.51
1:D:37:ALA:HB1	1:D:452:LEU:HD13	1.93	0.51
1:E:37:ALA:HB1	1:E:452:LEU:HD13	1.92	0.51
1:G:37:ALA:HB1	1:G:452:LEU:HD13	1.92	0.51
1:H:263:ARG:HB2	1:H:290:LEU:HB3	1.91	0.51
1:J:80:PRO:HA	1:J:83:PHE:HB2	1.92	0.51
1:A:37:ALA:HB1	1:A:452:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:TYR:CD2	1:I:185:CYS:HB2	2.46	0.51
1:I:37:ALA:HB1	1:I:452:LEU:HD13	1.93	0.51
1:A:263:ARG:HB2	1:A:290:LEU:HB3	1.91	0.51
1:C:459:ASP:OD1	1:C:459:ASP:N	2.43	0.51
1:E:253:GLU:HG3	1:F:113:LEU:HD12	1.92	0.51
1:F:152:LYS:NZ	1:F:202:ASP:OD2	2.37	0.51
1:G:152:LYS:HE3	1:G:253:GLU:HB2	1.93	0.51
1:A:256:PHE:HA	1:B:115:VAL:HG21	1.93	0.51
1:F:263:ARG:HB2	1:F:290:LEU:HB3	1.91	0.51
1:H:42:LEU:HB2	1:H:371:PHE:HB2	1.93	0.51
1:B:152:LYS:NZ	1:B:202:ASP:OD2	2.37	0.51
1:D:263:ARG:HB2	1:D:290:LEU:HB3	1.91	0.51
1:E:42:LEU:HB2	1:E:371:PHE:HB2	1.93	0.51
1:I:42:LEU:HB2	1:I:371:PHE:HB2	1.93	0.51
1:C:42:LEU:HB2	1:C:371:PHE:HB2	1.93	0.51
1:D:231:TYR:CD1	1:H:112:PRO:HB3	2.45	0.51
1:C:152:LYS:HE3	1:C:253:GLU:HB2	1.93	0.51
1:D:42:LEU:HB2	1:D:371:PHE:HB2	1.93	0.51
1:D:459:ASP:OD1	1:D:459:ASP:N	2.42	0.51
1:J:37:ALA:HB1	1:J:452:LEU:HD13	1.92	0.51
1:D:152:LYS:HE3	1:D:253:GLU:HB2	1.93	0.51
1:F:152:LYS:HE3	1:F:253:GLU:HB2	1.93	0.51
1:F:37:ALA:HB1	1:F:452:LEU:HD13	1.93	0.51
1:A:216:ASN:HB2	1:B:345:CYS:SG	2.50	0.50
1:I:152:LYS:HE3	1:I:253:GLU:HB2	1.92	0.50
1:H:459:ASP:OD1	1:H:459:ASP:N	2.42	0.50
1:H:80:PRO:HA	1:H:83:PHE:HB2	1.92	0.50
1:D:142:ASP:OD1	1:D:142:ASP:N	2.36	0.50
1:F:42:LEU:HB2	1:F:371:PHE:HB2	1.93	0.50
1:H:37:ALA:HB1	1:H:452:LEU:HD13	1.92	0.50
1:A:253:GLU:HG3	1:B:113:LEU:HD12	1.94	0.50
1:D:152:LYS:NZ	1:D:202:ASP:OD2	2.37	0.50
1:C:372:ASP:HB2	1:H:235:LEU:HD13	1.93	0.50
1:A:269:ASP:O	1:A:289:TYR:OH	2.21	0.50
1:C:37:ALA:HB1	1:C:452:LEU:HD13	1.93	0.50
1:F:80:PRO:HA	1:F:83:PHE:HB2	1.92	0.50
1:G:113:LEU:HD12	1:J:253:GLU:HG3	1.94	0.50
1:G:42:LEU:HB2	1:G:371:PHE:HB2	1.93	0.50
1:H:109:ARG:NE	1:H:335:ASP:OD2	2.38	0.50
1:J:42:LEU:HB2	1:J:371:PHE:HB2	1.93	0.50
1:E:231:TYR:CD1	1:F:112:PRO:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HB2	1:B:371:PHE:HB2	1.93	0.50
1:G:109:ARG:NE	1:G:335:ASP:OD2	2.38	0.50
1:H:152:LYS:HE3	1:H:253:GLU:HB2	1.93	0.50
1:E:109:ARG:NE	1:E:335:ASP:OD2	2.38	0.49
1:F:142:ASP:HB3	1:J:356:TYR:CE2	2.46	0.49
1:E:115:VAL:HG21	1:I:256:PHE:HA	1.93	0.49
1:B:152:LYS:HE3	1:B:253:GLU:HB2	1.93	0.49
1:J:109:ARG:NE	1:J:335:ASP:OD2	2.38	0.49
1:F:109:ARG:NE	1:F:335:ASP:OD2	2.38	0.49
1:B:269:ASP:O	1:B:289:TYR:OH	2.21	0.49
1:E:152:LYS:NZ	1:E:202:ASP:OD2	2.36	0.49
1:A:152:LYS:NZ	1:A:202:ASP:OD2	2.37	0.49
1:D:109:ARG:NE	1:D:335:ASP:OD2	2.38	0.49
1:B:463:PHE:O	1:B:467:ARG:HG3	2.13	0.49
1:C:149:VAL:HG21	1:C:294:SER:HB2	1.95	0.49
1:G:142:ASP:N	1:G:142:ASP:OD1	2.36	0.49
1:A:42:LEU:HB2	1:A:371:PHE:HB2	1.93	0.49
1:B:250:LEU:HB3	1:B:306:LEU:HD21	1.95	0.49
1:D:250:LEU:HB3	1:D:306:LEU:HD21	1.95	0.49
1:I:327:ASN:HD22	1:I:327:ASN:N	2.10	0.49
1:E:112:PRO:HB3	1:I:231:TYR:CD1	2.48	0.48
1:I:250:LEU:HB3	1:I:306:LEU:HD21	1.95	0.48
1:E:269:ASP:O	1:E:289:TYR:OH	2.21	0.48
1:G:250:LEU:HB3	1:G:306:LEU:HD21	1.95	0.48
1:H:250:LEU:HB3	1:H:306:LEU:HD21	1.95	0.48
1:F:235:LEU:HD13	1:J:372:ASP:HB2	1.96	0.48
1:E:250:LEU:HB3	1:E:306:LEU:HD21	1.96	0.48
1:A:149:VAL:HG21	1:A:294:SER:HB2	1.96	0.48
1:C:250:LEU:HB3	1:C:306:LEU:HD21	1.95	0.48
1:D:463:PHE:O	1:D:467:ARG:HG3	2.13	0.48
1:F:77:LEU:HB2	1:F:327:ASN:HB3	1.95	0.48
1:H:149:VAL:HG21	1:H:294:SER:HB2	1.96	0.48
1:H:92:ASP:OD1	1:H:94:ASN:ND2	2.40	0.48
1:A:77:LEU:HB2	1:A:327:ASN:HB3	1.95	0.48
1:F:149:VAL:HG21	1:F:294:SER:HB2	1.96	0.48
1:F:269:ASP:O	1:F:289:TYR:OH	2.21	0.48
1:H:77:LEU:HB2	1:H:327:ASN:HB3	1.95	0.48
1:B:109:ARG:NE	1:B:335:ASP:OD2	2.38	0.48
1:A:112:PRO:HB3	1:C:231:TYR:CD1	2.48	0.48
1:D:269:ASP:O	1:D:289:TYR:OH	2.21	0.48
1:F:459:ASP:OD1	1:F:459:ASP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLN:NE2	1:H:347:SER:O	2.41	0.48
1:A:142:ASP:N	1:A:142:ASP:OD1	2.36	0.48
1:F:185:CYS:HB2	1:J:364:TYR:CD2	2.49	0.48
1:G:142:ASP:HB3	1:I:356:TYR:CE2	2.49	0.48
1:J:250:LEU:HB3	1:J:306:LEU:HD21	1.95	0.48
1:A:250:LEU:HB3	1:A:306:LEU:HD21	1.95	0.48
1:C:327:ASN:HD22	1:C:327:ASN:N	2.12	0.48
1:E:149:VAL:HG21	1:E:294:SER:HB2	1.95	0.48
1:D:77:LEU:HB2	1:D:327:ASN:HB3	1.95	0.48
1:B:327:ASN:N	1:B:327:ASN:HD22	2.11	0.48
1:C:109:ARG:NE	1:C:335:ASP:OD2	2.38	0.48
1:E:113:LEU:HD12	1:I:253:GLU:HG3	1.96	0.48
1:B:149:VAL:HG21	1:B:294:SER:HB2	1.96	0.47
1:B:80:PRO:CD	1:B:327:ASN:OD1	2.62	0.47
1:G:152:LYS:NZ	1:G:202:ASP:OD2	2.37	0.47
1:G:269:ASP:O	1:G:289:TYR:OH	2.21	0.47
1:C:113:LEU:HD12	1:H:253:GLU:HG3	1.96	0.47
1:B:253:GLU:HG3	1:D:113:LEU:HD12	1.96	0.47
1:A:231:TYR:CD1	1:B:112:PRO:HB3	2.49	0.47
1:C:80:PRO:CD	1:C:327:ASN:OD1	2.62	0.47
1:D:156:LEU:HG	1:D:334:VAL:HB	1.96	0.47
1:I:149:VAL:HG21	1:I:294:SER:HB2	1.95	0.47
1:D:149:VAL:HG21	1:D:294:SER:HB2	1.95	0.47
1:A:459:ASP:N	1:A:459:ASP:OD1	2.42	0.47
1:G:58:GLY:HA2	1:G:59:ARG:HA	1.52	0.47
1:C:358:PRO:HG3	1:H:141:LYS:O	2.14	0.47
1:I:109:ARG:NE	1:I:335:ASP:OD2	2.38	0.47
1:J:149:VAL:HG21	1:J:294:SER:HB2	1.96	0.47
1:A:372:ASP:HB2	1:C:235:LEU:HD13	1.96	0.47
1:A:364:TYR:CZ	1:C:268:GLY:HA3	2.49	0.47
1:C:47:HIS:CE1	1:C:365:ALA:HB3	2.50	0.47
1:D:142:ASP:HB3	1:H:356:TYR:CE2	2.49	0.47
1:A:47:HIS:CE1	1:A:365:ALA:HB3	2.50	0.47
1:B:47:HIS:CE1	1:B:365:ALA:HB3	2.50	0.47
1:G:77:LEU:HB2	1:G:327:ASN:HB3	1.95	0.47
1:G:47:HIS:CE1	1:G:365:ALA:HB3	2.50	0.47
1:H:33:ILE:HB	1:H:379:LEU:HB3	1.97	0.47
1:I:80:PRO:CD	1:I:327:ASN:OD1	2.62	0.47
1:I:33:ILE:HB	1:I:379:LEU:HB3	1.97	0.47
1:J:77:LEU:HB2	1:J:327:ASN:HB3	1.95	0.47
1:B:231:TYR:CD1	1:D:112:PRO:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLY:HA2	1:C:59:ARG:HA	1.53	0.47
1:G:149:VAL:HG21	1:G:294:SER:HB2	1.95	0.47
1:C:112:PRO:HB3	1:H:231:TYR:CD1	2.50	0.47
1:C:33:ILE:HB	1:C:379:LEU:HB3	1.97	0.46
1:B:265:GLY:HA2	1:D:358:PRO:O	2.16	0.46
1:E:216:ASN:HB2	1:F:345:CYS:SG	2.55	0.46
1:F:250:LEU:HB3	1:F:306:LEU:HD21	1.97	0.46
1:H:269:ASP:O	1:H:289:TYR:OH	2.21	0.46
1:I:47:HIS:CE1	1:I:365:ALA:HB3	2.50	0.46
1:G:185:CYS:HB2	1:I:364:TYR:CD2	2.50	0.46
1:F:216:ASN:HB2	1:J:345:CYS:SG	2.55	0.46
1:J:47:HIS:CE1	1:J:365:ALA:HB3	2.50	0.46
1:A:185:CYS:HB2	1:B:364:TYR:CD2	2.50	0.46
1:C:269:ASP:O	1:C:289:TYR:OH	2.21	0.46
1:H:216:ASN:ND2	1:H:219:GLU:OE2	2.49	0.46
1:B:141:LYS:O	1:D:358:PRO:HG3	2.16	0.46
1:H:47:HIS:CE1	1:H:365:ALA:HB3	2.51	0.46
1:D:47:HIS:CE1	1:D:365:ALA:HB3	2.51	0.46
1:J:33:ILE:HB	1:J:379:LEU:HB3	1.97	0.46
1:A:33:ILE:HB	1:A:379:LEU:HB3	1.97	0.46
1:C:216:ASN:ND2	1:C:219:GLU:OE2	2.49	0.46
1:D:216:ASN:ND2	1:D:219:GLU:OE2	2.49	0.46
1:D:33:ILE:HB	1:D:379:LEU:HB3	1.98	0.46
1:G:33:ILE:HB	1:G:379:LEU:HB3	1.97	0.46
1:D:185:CYS:HB2	1:H:364:TYR:CD2	2.50	0.46
1:I:271:LEU:HD12	1:I:272:PRO:HD2	1.97	0.46
1:E:47:HIS:CE1	1:E:365:ALA:HB3	2.50	0.46
1:F:33:ILE:HB	1:F:379:LEU:HB3	1.97	0.46
1:G:372:ASP:HB2	1:J:235:LEU:HD13	1.98	0.46
1:G:112:PRO:HB3	1:J:231:TYR:CD1	2.51	0.46
1:E:33:ILE:HB	1:E:379:LEU:HB3	1.97	0.45
1:G:216:ASN:ND2	1:G:219:GLU:OE2	2.49	0.45
1:H:152:LYS:NZ	1:H:202:ASP:OD2	2.37	0.45
1:E:271:LEU:HD12	1:E:272:PRO:HD2	1.98	0.45
1:H:271:LEU:HD12	1:H:272:PRO:HD2	1.98	0.45
1:J:80:PRO:HD3	1:J:327:ASN:OD1	2.17	0.45
1:B:33:ILE:HB	1:B:379:LEU:HB3	1.97	0.45
1:E:235:LEU:HD13	1:F:372:ASP:HB2	1.98	0.45
1:E:258:ARG:HG2	1:E:259:HIS:CD2	2.52	0.45
1:H:80:PRO:HD3	1:H:327:ASN:OD1	2.16	0.45
1:A:258:ARG:HG2	1:A:259:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:ARG:HG2	1:F:259:HIS:CD2	2.52	0.45
1:H:258:ARG:HG2	1:H:259:HIS:CD2	2.52	0.45
1:E:216:ASN:ND2	1:E:219:GLU:OE2	2.49	0.45
1:F:216:ASN:ND2	1:F:219:GLU:OE2	2.49	0.45
1:G:80:PRO:HD3	1:G:327:ASN:OD1	2.17	0.45
1:J:258:ARG:HG2	1:J:259:HIS:CD2	2.52	0.45
1:A:271:LEU:HD12	1:A:272:PRO:HD2	1.98	0.45
1:D:271:LEU:HD12	1:D:272:PRO:HD2	1.98	0.45
1:F:47:HIS:CE1	1:F:365:ALA:HB3	2.50	0.45
1:G:258:ARG:HG2	1:G:259:HIS:CD2	2.52	0.45
1:G:271:LEU:HD12	1:G:272:PRO:HD2	1.98	0.45
1:G:345:CYS:SG	1:J:216:ASN:HB2	2.57	0.45
1:I:216:ASN:ND2	1:I:219:GLU:OE2	2.49	0.45
1:I:77:LEU:HB2	1:I:327:ASN:HB3	1.99	0.45
1:A:80:PRO:HD3	1:A:327:ASN:OD1	2.16	0.45
1:C:271:LEU:HD12	1:C:272:PRO:HD2	1.98	0.45
1:D:258:ARG:HG2	1:D:259:HIS:CD2	2.52	0.45
1:G:256:PHE:HA	1:I:115:VAL:HG21	1.99	0.45
1:I:258:ARG:HG2	1:I:259:HIS:CD2	2.52	0.45
1:A:216:ASN:ND2	1:A:219:GLU:OE2	2.49	0.44
1:F:271:LEU:HD12	1:F:272:PRO:HD2	1.98	0.44
1:I:113:LEU:HD22	1:I:337:THR:HB	2.00	0.44
1:B:113:LEU:HD22	1:B:337:THR:HB	2.00	0.44
1:B:258:ARG:HG2	1:B:259:HIS:CD2	2.52	0.44
1:F:80:PRO:HD3	1:F:327:ASN:OD1	2.16	0.44
1:J:216:ASN:ND2	1:J:219:GLU:OE2	2.49	0.44
1:B:58:GLY:HA2	1:B:59:ARG:HA	1.52	0.44
1:F:22:VAL:HG12	1:F:26:GLU:HG3	2.00	0.44
1:B:77:LEU:HB2	1:B:327:ASN:HB3	1.99	0.44
1:D:80:PRO:HD3	1:D:327:ASN:OD1	2.17	0.44
1:E:463:PHE:O	1:E:467:ARG:HG3	2.18	0.44
1:F:125:LYS:HB3	1:F:125:LYS:HE2	1.88	0.44
1:F:58:GLY:HA2	1:F:59:ARG:HA	1.46	0.44
1:I:269:ASP:O	1:I:289:TYR:OH	2.21	0.44
1:C:22:VAL:HG12	1:C:26:GLU:HG3	2.00	0.44
1:C:258:ARG:HG2	1:C:259:HIS:CD2	2.52	0.44
1:D:22:VAL:HG12	1:D:26:GLU:HG3	2.00	0.44
1:E:58:GLY:HA2	1:E:59:ARG:HA	1.52	0.44
1:D:216:ASN:HB2	1:H:345:CYS:SG	2.58	0.44
1:I:22:VAL:HG12	1:I:26:GLU:HG3	2.00	0.44
1:A:22:VAL:HG12	1:A:26:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:VAL:HG12	1:H:26:GLU:HG3	2.00	0.44
1:B:216:ASN:ND2	1:B:219:GLU:OE2	2.49	0.44
1:F:463:PHE:O	1:F:467:ARG:HG3	2.18	0.44
1:H:142:ASP:N	1:H:142:ASP:OD1	2.36	0.44
1:E:372:ASP:HB2	1:I:235:LEU:HD13	1.99	0.44
1:I:463:PHE:O	1:I:467:ARG:HG3	2.18	0.44
1:A:463:PHE:O	1:A:467:ARG:HG3	2.18	0.44
1:G:22:VAL:HG12	1:G:26:GLU:HG3	2.00	0.44
1:J:463:PHE:O	1:J:467:ARG:HG3	2.18	0.44
1:C:463:PHE:O	1:C:467:ARG:HG3	2.18	0.43
1:E:22:VAL:HG12	1:E:26:GLU:HG3	1.99	0.43
1:H:58:GLY:HA2	1:H:59:ARG:HA	1.52	0.43
1:G:176:LYS:HE3	1:I:59:ARG:HH21	1.83	0.43
1:F:182:GLN:NE2	1:J:347:SER:O	2.42	0.43
1:E:113:LEU:HD22	1:E:337:THR:HB	2.00	0.43
1:G:463:PHE:O	1:G:467:ARG:HG3	2.18	0.43
1:I:263:ARG:NE	1:I:292:SER:OG	2.52	0.43
1:H:92:ASP:OD2	1:I:386:THR:HG23	2.18	0.43
1:J:22:VAL:HG12	1:J:26:GLU:HG3	2.00	0.43
1:A:117:LEU:HD21	1:C:260:PHE:CD1	2.53	0.43
1:D:151:TYR:CG	1:D:203:THR:HB	2.54	0.43
1:G:263:ARG:NE	1:G:292:SER:OG	2.51	0.43
1:J:151:TYR:CG	1:J:203:THR:HB	2.53	0.43
1:G:364:TYR:CZ	1:J:268:GLY:HA3	2.53	0.43
1:J:271:LEU:HD12	1:J:272:PRO:HD2	1.98	0.43
1:C:151:TYR:CG	1:C:203:THR:HB	2.54	0.43
1:G:156:LEU:HG	1:G:334:VAL:HB	2.01	0.43
1:H:463:PHE:O	1:H:467:ARG:HG3	2.18	0.43
1:I:151:TYR:CG	1:I:203:THR:HB	2.54	0.43
1:C:364:TYR:CD2	1:H:185:CYS:HB2	2.54	0.43
1:D:263:ARG:NE	1:D:292:SER:OG	2.50	0.43
1:F:98:LEU:HD13	1:F:379:LEU:HD11	2.01	0.43
1:I:327:ASN:N	1:I:327:ASN:ND2	2.67	0.43
1:A:113:LEU:HD22	1:A:337:THR:HB	2.00	0.43
1:A:151:TYR:CG	1:A:203:THR:HB	2.54	0.43
1:A:263:ARG:NE	1:A:292:SER:OG	2.52	0.43
1:B:156:LEU:HG	1:B:334:VAL:HB	2.01	0.43
1:B:22:VAL:HG12	1:B:26:GLU:HG3	2.00	0.43
1:C:77:LEU:HB2	1:C:327:ASN:HB3	1.99	0.43
1:D:113:LEU:HD22	1:D:337:THR:HB	2.00	0.43
1:F:263:ARG:NE	1:F:292:SER:OG	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:LEU:HD13	1:J:379:LEU:HD11	2.01	0.43
1:A:149:VAL:HA	1:C:260:PHE:CE2	2.54	0.43
1:B:271:LEU:HD12	1:B:272:PRO:HD2	1.99	0.43
1:B:442:TYR:HB3	1:B:447:PHE:HE2	1.84	0.43
1:E:247:PHE:HB2	1:E:316:ALA:CB	2.48	0.43
1:F:151:TYR:CG	1:F:203:THR:HB	2.53	0.43
1:G:393:HIS:CD2	1:G:397:THR:HG23	2.54	0.43
1:H:113:LEU:HD22	1:H:337:THR:HB	2.00	0.43
1:H:151:TYR:CG	1:H:203:THR:HB	2.54	0.43
1:H:247:PHE:HB2	1:H:316:ALA:CB	2.47	0.43
1:H:263:ARG:NE	1:H:292:SER:OG	2.52	0.43
1:D:442:TYR:HB3	1:D:447:PHE:HE2	1.84	0.43
1:C:358:PRO:HG3	1:H:141:LYS:C	2.38	0.43
1:I:156:LEU:HG	1:I:334:VAL:HB	2.01	0.43
1:B:268:GLY:HA3	1:D:364:TYR:CZ	2.54	0.43
1:B:305:GLN:OE1	1:B:338:ARG:NH1	2.39	0.43
1:C:263:ARG:NE	1:C:292:SER:OG	2.52	0.43
1:E:156:LEU:HG	1:E:334:VAL:HB	2.01	0.43
1:E:98:LEU:HD13	1:E:379:LEU:HD11	2.01	0.43
1:F:113:LEU:HD22	1:F:337:THR:HB	2.00	0.43
1:G:105:VAL:HG21	1:G:159:ILE:HD13	2.01	0.43
1:H:98:LEU:HD13	1:H:379:LEU:HD11	2.01	0.43
1:J:113:LEU:HD22	1:J:337:THR:HB	2.00	0.43
1:J:247:PHE:HB2	1:J:316:ALA:CB	2.48	0.43
1:A:105:VAL:HG21	1:A:159:ILE:HD13	2.01	0.43
1:A:247:PHE:HB2	1:A:316:ALA:CB	2.48	0.43
1:B:158:ILE:HB	1:B:332:THR:HB	2.01	0.43
1:C:113:LEU:HD22	1:C:337:THR:HB	2.00	0.43
1:E:185:CYS:HB2	1:F:364:TYR:CD2	2.53	0.43
1:F:393:HIS:CD2	1:F:397:THR:HG23	2.54	0.43
1:G:151:TYR:CG	1:G:203:THR:HB	2.54	0.43
1:H:105:VAL:HG21	1:H:159:ILE:HD13	2.01	0.43
1:H:156:LEU:HG	1:H:334:VAL:HB	2.00	0.43
1:H:393:HIS:CD2	1:H:397:THR:HG23	2.54	0.43
1:J:105:VAL:HG21	1:J:159:ILE:HD13	2.01	0.43
1:J:158:ILE:HB	1:J:332:THR:HB	2.01	0.43
1:J:263:ARG:NE	1:J:292:SER:OG	2.52	0.43
1:B:263:ARG:NE	1:B:292:SER:OG	2.52	0.42
1:C:247:PHE:HB2	1:C:316:ALA:CB	2.48	0.42
1:D:158:ILE:HB	1:D:332:THR:HB	2.01	0.42
1:D:105:VAL:HG21	1:D:159:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:GLY:HA2	1:D:247:PHE:CE2	2.55	0.42
1:D:393:HIS:CD2	1:D:397:THR:HG23	2.54	0.42
1:E:393:HIS:CD2	1:E:397:THR:HG23	2.54	0.42
1:G:113:LEU:HD22	1:G:337:THR:HB	2.00	0.42
1:G:158:ILE:HB	1:G:332:THR:HB	2.01	0.42
1:J:442:TYR:HB3	1:J:447:PHE:HE2	1.84	0.42
1:A:235:LEU:HD13	1:B:372:ASP:HB2	1.99	0.42
1:B:151:TYR:CG	1:B:203:THR:HB	2.54	0.42
1:B:366:ARG:HD3	1:B:366:ARG:HA	1.92	0.42
1:B:98:LEU:HD13	1:B:379:LEU:HD11	2.01	0.42
1:D:235:LEU:HD13	1:H:372:ASP:HB2	2.00	0.42
1:E:347:SER:O	1:I:182:GLN:NE2	2.44	0.42
1:H:160:GLY:HA2	1:H:247:PHE:CE2	2.54	0.42
1:I:158:ILE:HB	1:I:332:THR:HB	2.01	0.42
1:I:442:TYR:HB3	1:I:447:PHE:HE2	1.84	0.42
1:B:125:LYS:HB3	1:B:125:LYS:HE2	1.88	0.42
1:B:327:ASN:N	1:B:327:ASN:ND2	2.67	0.42
1:C:393:HIS:CD2	1:C:397:THR:HG23	2.54	0.42
1:D:247:PHE:HB2	1:D:316:ALA:CB	2.47	0.42
1:E:364:TYR:CE2	1:I:185:CYS:HB2	2.54	0.42
1:I:98:LEU:HD13	1:I:379:LEU:HD11	2.01	0.42
1:A:158:ILE:HB	1:A:332:THR:HB	2.01	0.42
1:C:160:GLY:HA2	1:C:247:PHE:CE2	2.55	0.42
1:E:366:ARG:HA	1:E:366:ARG:HD3	1.91	0.42
1:F:158:ILE:HB	1:F:332:THR:HB	2.01	0.42
1:G:68:TYR:CE1	1:G:151:TYR:HB2	2.55	0.42
1:J:160:GLY:HA2	1:J:247:PHE:CE2	2.55	0.42
1:J:156:LEU:HG	1:J:334:VAL:HB	2.01	0.42
1:E:151:TYR:CG	1:E:203:THR:HB	2.54	0.42
1:E:263:ARG:NE	1:E:292:SER:OG	2.52	0.42
1:F:156:LEU:HG	1:F:334:VAL:HB	2.00	0.42
1:I:105:VAL:HG21	1:I:159:ILE:HD13	2.02	0.42
1:A:393:HIS:CD2	1:A:397:THR:HG23	2.54	0.42
1:A:442:TYR:HB3	1:A:447:PHE:HE2	1.84	0.42
1:D:98:LEU:HD13	1:D:379:LEU:HD11	2.01	0.42
1:F:442:TYR:HB3	1:F:447:PHE:HE2	1.84	0.42
1:J:366:ARG:HA	1:J:366:ARG:HD3	1.91	0.42
1:J:68:TYR:CE1	1:J:151:TYR:HB2	2.55	0.42
1:A:156:LEU:HG	1:A:334:VAL:HB	2.00	0.42
1:A:98:LEU:HD13	1:A:379:LEU:HD11	2.01	0.42
1:A:68:TYR:CE1	1:A:151:TYR:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD12	1:B:365:ALA:HB2	2.02	0.42
1:E:442:TYR:HB3	1:E:447:PHE:HE2	1.84	0.42
1:H:442:TYR:HB3	1:H:447:PHE:HE2	1.84	0.42
1:I:68:TYR:CE1	1:I:151:TYR:HB2	2.55	0.42
1:B:105:VAL:HG21	1:B:159:ILE:HD13	2.01	0.42
1:B:160:GLY:HA2	1:B:247:PHE:CE2	2.55	0.42
1:C:156:LEU:HG	1:C:334:VAL:HB	2.01	0.42
1:F:68:TYR:CE1	1:F:151:TYR:HB2	2.55	0.42
1:G:208:MET:SD	1:I:342:LEU:HD22	2.60	0.42
1:J:125:LYS:HB3	1:J:125:LYS:HE2	1.88	0.42
1:G:358:PRO:HG3	1:J:141:LYS:O	2.19	0.42
1:F:260:PHE:CE2	1:J:149:VAL:HA	2.55	0.42
1:B:460:LEU:HD12	1:B:470:LEU:HD21	2.02	0.42
1:G:160:GLY:HA2	1:G:247:PHE:CE2	2.55	0.42
1:F:185:CYS:HB2	1:J:364:TYR:CE2	2.55	0.42
1:A:160:GLY:HA2	1:A:247:PHE:CE2	2.55	0.42
1:E:158:ILE:HB	1:E:332:THR:HB	2.01	0.42
1:E:460:LEU:HD12	1:E:470:LEU:HD21	2.02	0.42
1:I:393:HIS:CD2	1:I:397:THR:HG23	2.54	0.42
1:A:460:LEU:HD12	1:A:470:LEU:HD21	2.02	0.41
1:G:291:TYR:CD1	1:I:148:SER:HB3	2.55	0.41
1:H:158:ILE:HB	1:H:332:THR:HB	2.01	0.41
1:I:68:TYR:CZ	1:I:151:TYR:HB2	2.55	0.41
1:E:141:LYS:O	1:F:358:PRO:HG3	2.20	0.41
1:F:68:TYR:CZ	1:F:151:TYR:HB2	2.55	0.41
1:F:460:LEU:HD12	1:F:470:LEU:HD21	2.02	0.41
1:H:398:THR:HA	1:H:401:GLU:HB2	2.02	0.41
1:H:396:ASN:HB3	1:H:399:ILE:HG13	2.02	0.41
1:I:247:PHE:HB2	1:I:316:ALA:CB	2.47	0.41
1:J:68:TYR:CZ	1:J:151:TYR:HB2	2.56	0.41
1:D:216:ASN:HD22	1:D:219:GLU:HG2	1.86	0.41
1:E:68:TYR:CZ	1:E:151:TYR:HB2	2.55	0.41
1:F:160:GLY:HA2	1:F:247:PHE:CE2	2.55	0.41
1:I:160:GLY:HA2	1:I:247:PHE:CE2	2.55	0.41
1:I:396:ASN:HB3	1:I:399:ILE:HG13	2.02	0.41
1:A:68:TYR:CZ	1:A:151:TYR:HB2	2.55	0.41
1:A:398:THR:HA	1:A:401:GLU:HB2	2.02	0.41
1:B:68:TYR:CZ	1:B:151:TYR:HB2	2.55	0.41
1:C:68:TYR:CE1	1:C:151:TYR:HB2	2.55	0.41
1:C:366:ARG:HA	1:C:366:ARG:HD3	1.92	0.41
1:D:68:TYR:CZ	1:D:151:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:SER:HB3	1:I:291:TYR:CD1	2.56	0.41
1:E:160:GLY:HA2	1:E:247:PHE:CE2	2.55	0.41
1:E:68:TYR:CE1	1:E:151:TYR:HB2	2.55	0.41
1:F:105:VAL:HG21	1:F:159:ILE:HD13	2.01	0.41
1:G:125:LYS:HE2	1:G:125:LYS:HB3	1.88	0.41
1:G:460:LEU:HD12	1:G:470:LEU:HD21	2.02	0.41
1:G:182:GLN:NE2	1:I:347:SER:O	2.42	0.41
1:B:393:HIS:CD2	1:B:397:THR:HG23	2.54	0.41
1:B:68:TYR:CE1	1:B:151:TYR:HB2	2.55	0.41
1:C:158:ILE:HB	1:C:332:THR:HB	2.01	0.41
1:E:105:VAL:HG21	1:E:159:ILE:HD13	2.01	0.41
1:E:265:GLY:HA2	1:F:358:PRO:O	2.20	0.41
1:G:271:LEU:HA	1:G:272:PRO:HD3	1.92	0.41
1:G:442:TYR:HB3	1:G:447:PHE:HE2	1.84	0.41
1:B:396:ASN:HB3	1:B:399:ILE:HG13	2.02	0.41
1:C:442:TYR:HB3	1:C:447:PHE:HE2	1.84	0.41
1:G:185:CYS:HB2	1:I:364:TYR:CG	2.56	0.41
1:G:396:ASN:HB3	1:G:399:ILE:HG13	2.02	0.41
1:H:216:ASN:HD22	1:H:219:GLU:HG2	1.86	0.41
1:H:68:TYR:CE1	1:H:151:TYR:HB2	2.55	0.41
1:E:217:LYS:HB2	1:I:277:ILE:HG13	2.02	0.41
1:J:393:HIS:CD2	1:J:397:THR:HG23	2.54	0.41
1:B:216:ASN:HD22	1:B:219:GLU:HG2	1.85	0.41
1:C:105:VAL:HG21	1:C:159:ILE:HD13	2.01	0.41
1:C:98:LEU:HD13	1:C:379:LEU:HD11	2.01	0.41
1:C:460:LEU:HD12	1:C:470:LEU:HD21	2.02	0.41
1:B:216:ASN:HB2	1:D:345:CYS:SG	2.60	0.41
1:D:58:GLY:HA2	1:D:59:ARG:HA	1.52	0.41
1:G:68:TYR:CZ	1:G:151:TYR:HB2	2.55	0.41
1:B:247:PHE:HB2	1:B:316:ALA:CB	2.47	0.41
1:D:68:TYR:CE1	1:D:151:TYR:HB2	2.55	0.41
1:E:216:ASN:HD22	1:E:219:GLU:HG2	1.85	0.41
1:F:67:ALA:HB2	1:F:367:HIS:NE2	2.36	0.41
1:G:216:ASN:HD22	1:G:219:GLU:HG2	1.85	0.41
1:E:185:CYS:HB2	1:F:364:TYR:CE2	2.56	0.41
1:F:305:GLN:OE1	1:F:338:ARG:NH1	2.39	0.41
1:G:98:LEU:HD13	1:G:379:LEU:HD11	2.01	0.41
1:C:364:TYR:CZ	1:H:268:GLY:HA3	2.56	0.41
1:H:67:ALA:HB2	1:H:367:HIS:NE2	2.36	0.41
1:I:125:LYS:HE2	1:I:125:LYS:HB3	1.88	0.41
1:A:305:GLN:OE1	1:A:338:ARG:NH1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LYS:HB3	1:C:125:LYS:HE2	1.88	0.41
1:C:68:TYR:CZ	1:C:151:TYR:HB2	2.55	0.41
1:C:327:ASN:ND2	1:C:327:ASN:N	2.67	0.41
1:C:43:LEU:HD11	1:H:190:LEU:HD23	2.01	0.41
1:D:366:ARG:HA	1:D:366:ARG:HD3	1.92	0.41
1:E:398:THR:HA	1:E:401:GLU:HB2	2.03	0.41
1:F:216:ASN:HD22	1:F:219:GLU:HG2	1.86	0.41
1:G:398:THR:HA	1:G:401:GLU:HB2	2.03	0.41
1:G:364:TYR:CD2	1:J:185:CYS:HB2	2.56	0.41
1:A:58:GLY:HA2	1:A:59:ARG:HA	1.52	0.41
1:F:396:ASN:HB3	1:F:399:ILE:HG13	2.02	0.41
1:D:185:CYS:HB2	1:H:364:TYR:CE2	2.56	0.41
1:J:67:ALA:HB2	1:J:367:HIS:NE2	2.36	0.41
1:B:263:ARG:HG3	1:B:290:LEU:HD23	2.03	0.40
1:C:271:LEU:HA	1:C:272:PRO:HD3	1.92	0.40
1:C:396:ASN:HB3	1:C:399:ILE:HG13	2.02	0.40
1:D:396:ASN:HB3	1:D:399:ILE:HG13	2.02	0.40
1:H:460:LEU:HD12	1:H:470:LEU:HD21	2.02	0.40
1:F:260:PHE:CD1	1:J:117:LEU:HD21	2.56	0.40
1:A:216:ASN:HD22	1:A:219:GLU:HG2	1.85	0.40
1:A:176:LYS:HE3	1:B:59:ARG:HH21	1.85	0.40
1:C:398:THR:HA	1:C:401:GLU:HB2	2.03	0.40
1:C:365:ALA:HB2	1:H:290:LEU:HD12	2.03	0.40
1:I:460:LEU:HD12	1:I:470:LEU:HD21	2.02	0.40
1:J:271:LEU:HA	1:J:272:PRO:HD3	1.92	0.40
1:J:396:ASN:HB3	1:J:399:ILE:HG13	2.02	0.40
1:C:216:ASN:HD22	1:C:219:GLU:HG2	1.85	0.40
1:E:59:ARG:HH21	1:I:176:LYS:HE3	1.87	0.40
1:F:66:SER:O	1:F:69:GLN:HG2	2.22	0.40
1:G:67:ALA:HB2	1:G:367:HIS:NE2	2.36	0.40
1:I:216:ASN:HD22	1:I:219:GLU:HG2	1.86	0.40
1:J:460:LEU:HD12	1:J:470:LEU:HD21	2.02	0.40
1:A:66:SER:O	1:A:69:GLN:HG2	2.22	0.40
1:B:398:THR:HA	1:B:401:GLU:HB2	2.02	0.40
1:B:66:SER:O	1:B:69:GLN:HG2	2.22	0.40
1:C:67:ALA:HB2	1:C:367:HIS:NE2	2.36	0.40
1:D:398:THR:HA	1:D:401:GLU:HB2	2.03	0.40
1:D:66:SER:O	1:D:69:GLN:HG2	2.22	0.40
1:E:396:ASN:HB3	1:E:399:ILE:HG13	2.02	0.40
1:F:271:LEU:HA	1:F:272:PRO:HD3	1.91	0.40
1:J:216:ASN:HD22	1:J:219:GLU:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:HB2	1:A:367:HIS:NE2	2.36	0.40
1:B:235:LEU:HD13	1:D:372:ASP:HB2	2.02	0.40
1:F:398:THR:HA	1:F:401:GLU:HB2	2.02	0.40
1:G:66:SER:O	1:G:69:GLN:HG2	2.22	0.40
1:D:260:PHE:CE2	1:H:149:VAL:HA	2.57	0.40
1:H:68:TYR:CZ	1:H:151:TYR:HB2	2.55	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:G:173:THR:OG1	1:J:57:ASN:O[2_547]	1.85	0.35
1:D:280:THR:OG1	1:I:141:LYS:NZ[1_554]	1.95	0.25
1:F:57:ASN:ND2	1:I:386:THR:OG1[2_657]	2.15	0.05
1:F:57:ASN:ND2	1:H:88:ASN:OD1[2_657]	2.16	0.04

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	416/500 (83%)	376 (90%)	36 (9%)	4 (1%)	18	61
1	B	410/500 (82%)	372 (91%)	35 (8%)	3 (1%)	25	68
1	C	416/500 (83%)	376 (90%)	36 (9%)	4 (1%)	18	61
1	D	416/500 (83%)	376 (90%)	36 (9%)	4 (1%)	18	61
1	E	416/500 (83%)	376 (90%)	36 (9%)	4 (1%)	18	61
1	F	416/500 (83%)	374 (90%)	37 (9%)	5 (1%)	15	58
1	G	416/500 (83%)	376 (90%)	36 (9%)	4 (1%)	18	61
1	H	408/500 (82%)	370 (91%)	35 (9%)	3 (1%)	25	68
1	I	416/500 (83%)	376 (90%)	36 (9%)	4 (1%)	18	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	416/500 (83%)	376 (90%)	36 (9%)	4 (1%)	18	61
All	All	4146/5000 (83%)	3748 (90%)	359 (9%)	39 (1%)	20	63

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	B	130	GLU
1	C	130	GLU
1	D	130	GLU
1	E	130	GLU
1	F	130	GLU
1	G	130	GLU
1	H	130	GLU
1	I	130	GLU
1	J	130	GLU
1	A	133	HIS
1	B	133	HIS
1	C	133	HIS
1	D	133	HIS
1	E	133	HIS
1	F	133	HIS
1	G	133	HIS
1	H	133	HIS
1	I	133	HIS
1	J	133	HIS
1	A	124	ASN
1	B	124	ASN
1	C	124	ASN
1	D	124	ASN
1	E	124	ASN
1	F	124	ASN
1	G	124	ASN
1	H	124	ASN
1	I	124	ASN
1	J	124	ASN
1	D	177	PRO
1	A	177	PRO
1	C	177	PRO
1	E	177	PRO
1	F	56	GLY
1	F	177	PRO

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Mol	Chain	Res	Type
1	G	177	PRO
1	I	177	PRO
1	J	177	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/444 (85%)	370 (98%)	6 (2%)	68	86
1	B	372/444 (84%)	365 (98%)	7 (2%)	62	83
1	C	376/444 (85%)	370 (98%)	6 (2%)	68	86
1	D	376/444 (85%)	371 (99%)	5 (1%)	73	88
1	E	376/444 (85%)	371 (99%)	5 (1%)	73	88
1	F	376/444 (85%)	371 (99%)	5 (1%)	73	88
1	G	376/444 (85%)	371 (99%)	5 (1%)	73	88
1	H	371/444 (84%)	367 (99%)	4 (1%)	78	89
1	I	376/444 (85%)	370 (98%)	6 (2%)	68	86
1	J	376/444 (85%)	371 (99%)	5 (1%)	73	88
All	All	3751/4440 (84%)	3697 (99%)	54 (1%)	71	87

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	VAL
1	A	173	THR
1	A	256	PHE
1	A	264	SER
1	A	306	LEU
1	A	396	ASN
1	B	134	VAL
1	B	173	THR
1	B	256	PHE
1	B	264	SER

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Mol	Chain	Res	Type
1	B	306	LEU
1	B	327	ASN
1	B	396	ASN
1	C	173	THR
1	C	256	PHE
1	C	264	SER
1	C	306	LEU
1	C	327	ASN
1	C	396	ASN
1	D	173	THR
1	D	256	PHE
1	D	264	SER
1	D	306	LEU
1	D	396	ASN
1	E	173	THR
1	E	256	PHE
1	E	264	SER
1	E	306	LEU
1	E	396	ASN
1	F	173	THR
1	F	256	PHE
1	F	264	SER
1	F	306	LEU
1	F	396	ASN
1	G	173	THR
1	G	256	PHE
1	G	264	SER
1	G	306	LEU
1	G	396	ASN
1	H	256	PHE
1	H	264	SER
1	H	306	LEU
1	H	396	ASN
1	I	173	THR
1	I	256	PHE
1	I	264	SER
1	I	306	LEU
1	I	327	ASN
1	I	396	ASN
1	J	173	THR
1	J	256	PHE
1	J	264	SER

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Mol	Chain	Res	Type
1	J	306	LEU
1	J	396	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	216	ASN
1	B	47	HIS
1	B	216	ASN
1	C	47	HIS
1	C	216	ASN
1	D	47	HIS
1	D	216	ASN
1	E	47	HIS
1	F	47	HIS
1	F	216	ASN
1	G	47	HIS
1	G	216	ASN
1	H	47	HIS
1	H	216	ASN
1	I	47	HIS
1	I	216	ASN
1	J	47	HIS
1	J	216	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

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	420/500 (84%)	-0.10	2 (0%) 90 86	77, 114, 203, 264	0
1	B	416/500 (83%)	-0.08	2 (0%) 90 86	78, 113, 187, 265	0
1	C	420/500 (84%)	-0.08	7 (1%) 70 61	78, 113, 202, 265	0
1	D	420/500 (84%)	-0.02	2 (0%) 90 86	78, 114, 203, 264	0
1	E	420/500 (84%)	-0.09	8 (1%) 67 58	78, 114, 202, 265	0
1	F	420/500 (84%)	0.06	9 (2%) 64 54	81, 114, 205, 265	0
1	G	420/500 (84%)	-0.08	6 (1%) 75 66	77, 114, 206, 264	0
1	H	414/500 (82%)	-0.01	6 (1%) 75 66	80, 114, 187, 265	0
1	I	420/500 (84%)	0.01	5 (1%) 79 71	79, 114, 202, 265	0
1	J	420/500 (84%)	-0.06	7 (1%) 70 61	78, 114, 202, 269	0
All	All	4190/5000 (83%)	-0.05	54 (1%) 77 68	77, 114, 202, 269	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	175	SER	6.6
1	J	175	SER	5.0
1	F	57	ASN	4.7
1	E	57	ASN	4.6
1	C	175	SER	4.5
1	I	141	LYS	4.1
1	F	56	GLY	3.8
1	C	177	PRO	3.6
1	F	58	GLY	3.6
1	C	176	LYS	3.5
1	F	171	LYS	3.3
1	J	174	ALA	3.3
1	F	55	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	58	GLY	3.1
1	G	176	LYS	3.0
1	E	88	ASN	2.9
1	E	175	SER	2.9
1	G	85	LEU	2.8
1	J	87	ASP	2.8
1	A	362	LYS	2.8
1	J	177	PRO	2.7
1	J	179	THR	2.7
1	E	278	LYS	2.5
1	I	173	THR	2.5
1	C	178	THR	2.5
1	G	287	GLY	2.5
1	E	56	GLY	2.5
1	J	176	LYS	2.5
1	D	439	GLN	2.4
1	I	59	ARG	2.4
1	H	346	ALA	2.4
1	E	277	ILE	2.4
1	H	133	HIS	2.3
1	G	87	ASP	2.3
1	H	348	THR	2.2
1	B	56	GLY	2.2
1	F	170	THR	2.2
1	C	180	VAL	2.2
1	B	279	GLY	2.2
1	G	174	ALA	2.2
1	H	354	ASN	2.2
1	H	347	SER	2.2
1	I	174	ALA	2.2
1	I	363	GLU	2.1
1	A	59	ARG	2.1
1	D	122	LEU	2.1
1	C	171	LYS	2.1
1	F	175	SER	2.1
1	E	383	THR	2.1
1	C	174	ALA	2.1
1	F	211	LYS	2.0
1	H	243	GLY	2.0
1	J	348	THR	2.0
1	F	132	SER	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.