



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:46 PM UTC

PDB ID : 2R5K / pdb_00002r5k
Title : Pentamer Structure of Major Capsid protein L1 of Human Papilloma Virus type 11
Authors : Bishop, B.; Dasgupta, J.; Chen, X.S.
Deposited on : 2007-09-03
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

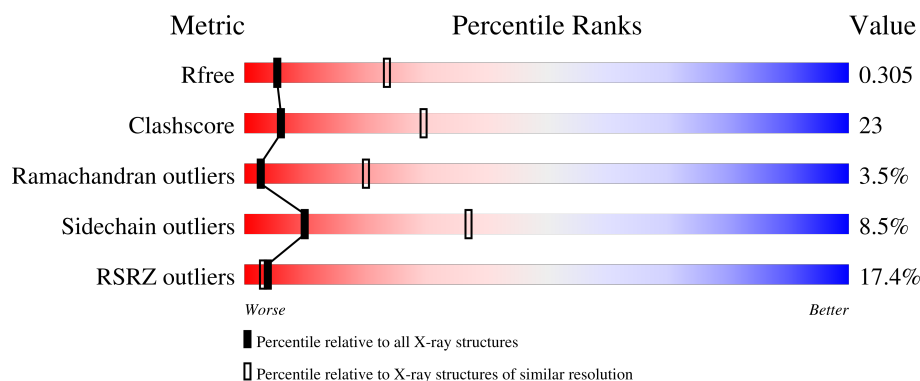
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	424	17% 54% 38% 7%
1	B	424	16% 53% 39% 6%
1	C	424	17% 54% 37% 7%
1	D	424	18% 54% 38% 7%
1	E	424	18% 51% 40% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16390 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	419	Total	C	N	O	S	0	0	0
			3278	2076	554	628	20			
1	B	419	Total	C	N	O	S	0	0	0
			3278	2076	554	628	20			
1	C	419	Total	C	N	O	S	0	0	0
			3278	2076	554	628	20			
1	D	419	Total	C	N	O	S	0	0	0
			3278	2076	554	628	20			
1	E	419	Total	C	N	O	S	0	0	0
			3278	2076	554	628	20			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	-	expression tag	UNP P04012
A	172	SER	CYS	engineered mutation	UNP P04012
A	327	SER	PHE	engineered mutation	UNP P04012
A	400	GLY	-	linker	UNP P04012
A	401	GLY	-	linker	UNP P04012
A	402	SER	-	linker	UNP P04012
A	403	GLY	-	linker	UNP P04012
A	404	GLY	-	linker	UNP P04012
B	19	ALA	-	expression tag	UNP P04012
B	172	SER	CYS	engineered mutation	UNP P04012
B	327	SER	PHE	engineered mutation	UNP P04012
B	400	GLY	-	linker	UNP P04012
B	401	GLY	-	linker	UNP P04012
B	402	SER	-	linker	UNP P04012
B	403	GLY	-	linker	UNP P04012
B	404	GLY	-	linker	UNP P04012
C	19	ALA	-	expression tag	UNP P04012
C	172	SER	CYS	engineered mutation	UNP P04012
C	327	SER	PHE	engineered mutation	UNP P04012

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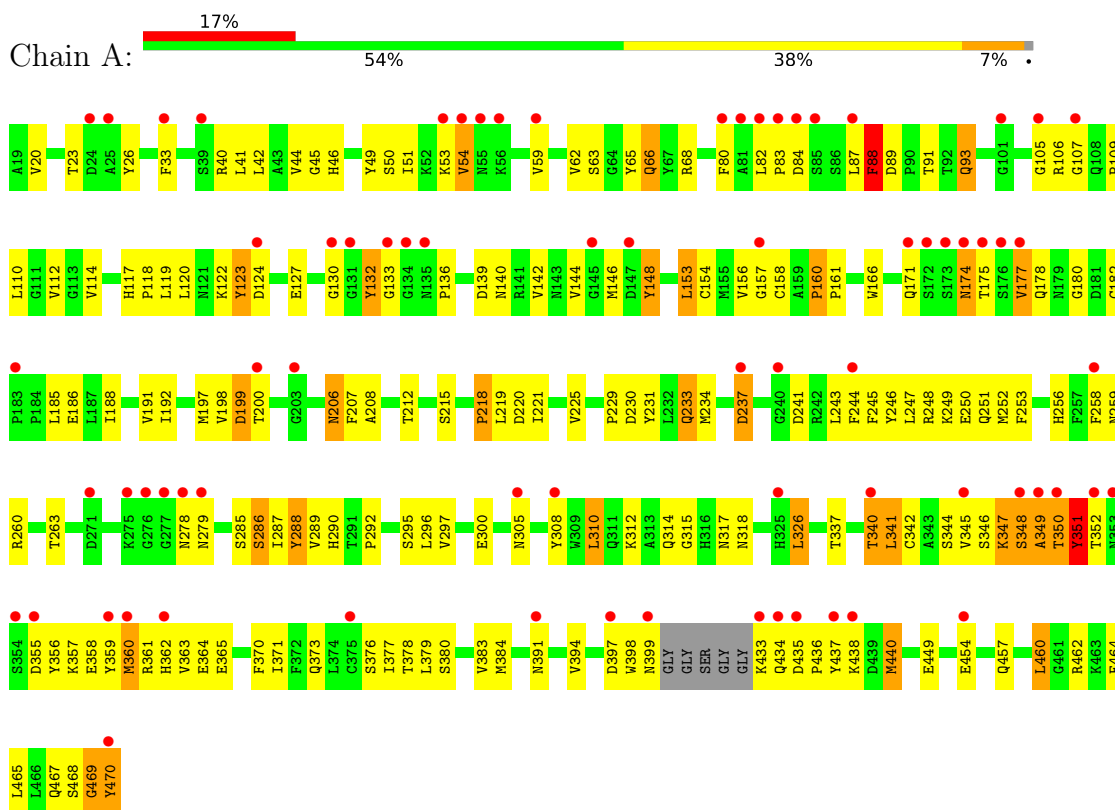
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Chain	Residue	Modelled	Actual	Comment	Reference
C	400	GLY	-	linker	UNP P04012
C	401	GLY	-	linker	UNP P04012
C	402	SER	-	linker	UNP P04012
C	403	GLY	-	linker	UNP P04012
C	404	GLY	-	linker	UNP P04012
D	19	ALA	-	expression tag	UNP P04012
D	172	SER	CYS	engineered mutation	UNP P04012
D	327	SER	PHE	engineered mutation	UNP P04012
D	400	GLY	-	linker	UNP P04012
D	401	GLY	-	linker	UNP P04012
D	402	SER	-	linker	UNP P04012
D	403	GLY	-	linker	UNP P04012
D	404	GLY	-	linker	UNP P04012
E	19	ALA	-	expression tag	UNP P04012
E	172	SER	CYS	engineered mutation	UNP P04012
E	327	SER	PHE	engineered mutation	UNP P04012
E	400	GLY	-	linker	UNP P04012
E	401	GLY	-	linker	UNP P04012
E	402	SER	-	linker	UNP P04012
E	403	GLY	-	linker	UNP P04012
E	404	GLY	-	linker	UNP P04012

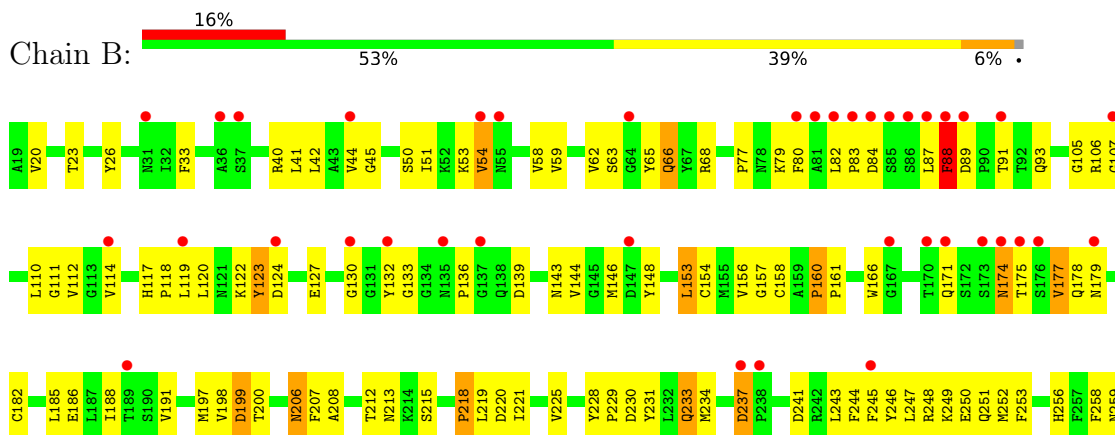
3 Residue-property plots [i](#)

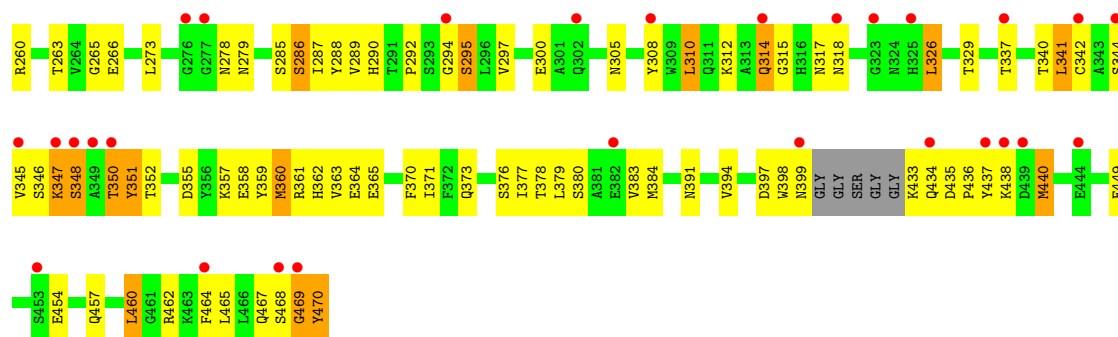
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Major capsid protein L1

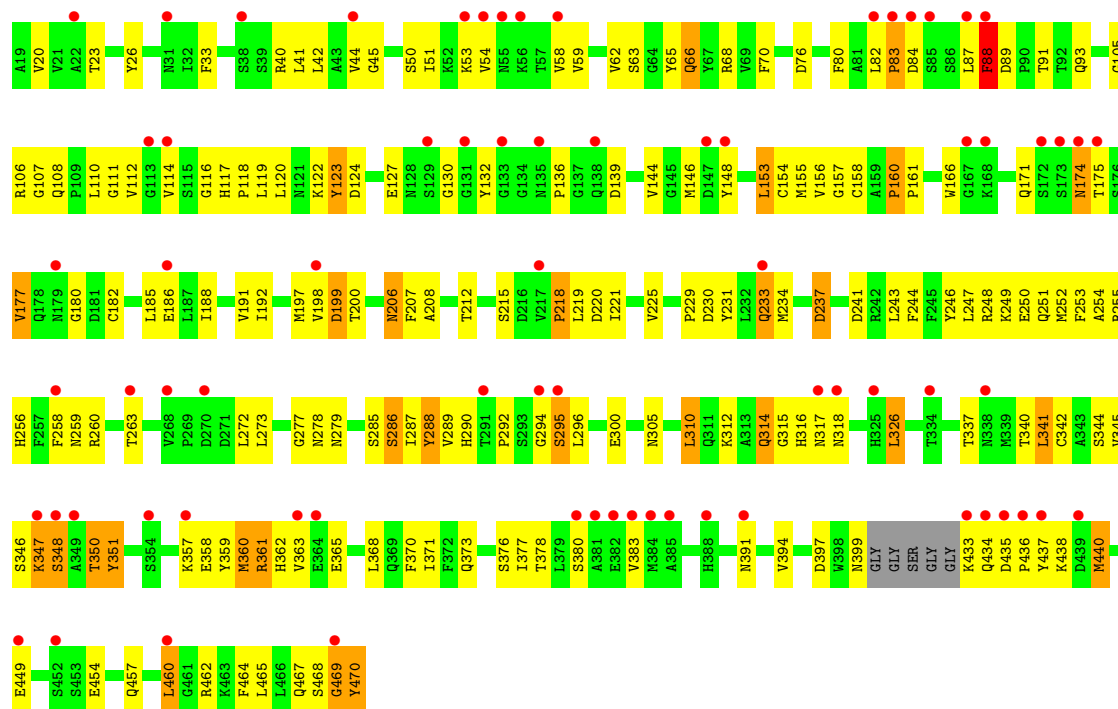


• Molecule 1: Major capsid protein L1

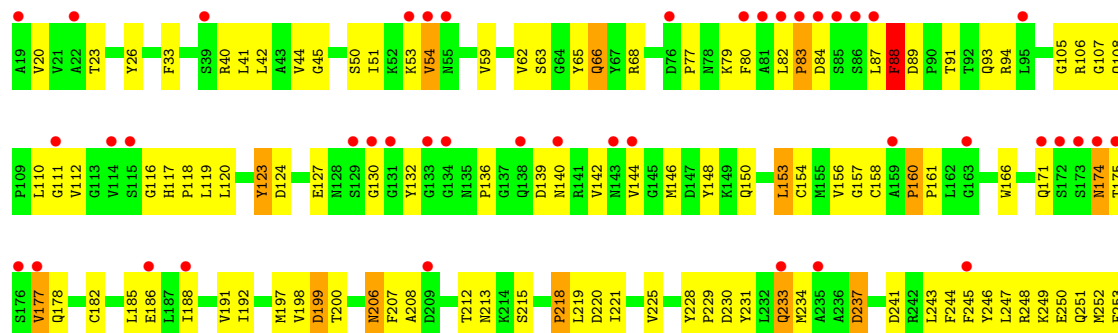


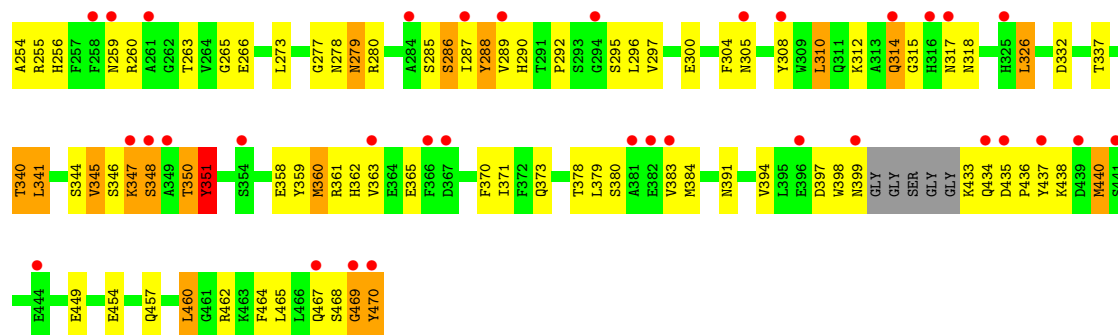


• Molecule 1: Major capsid protein L1

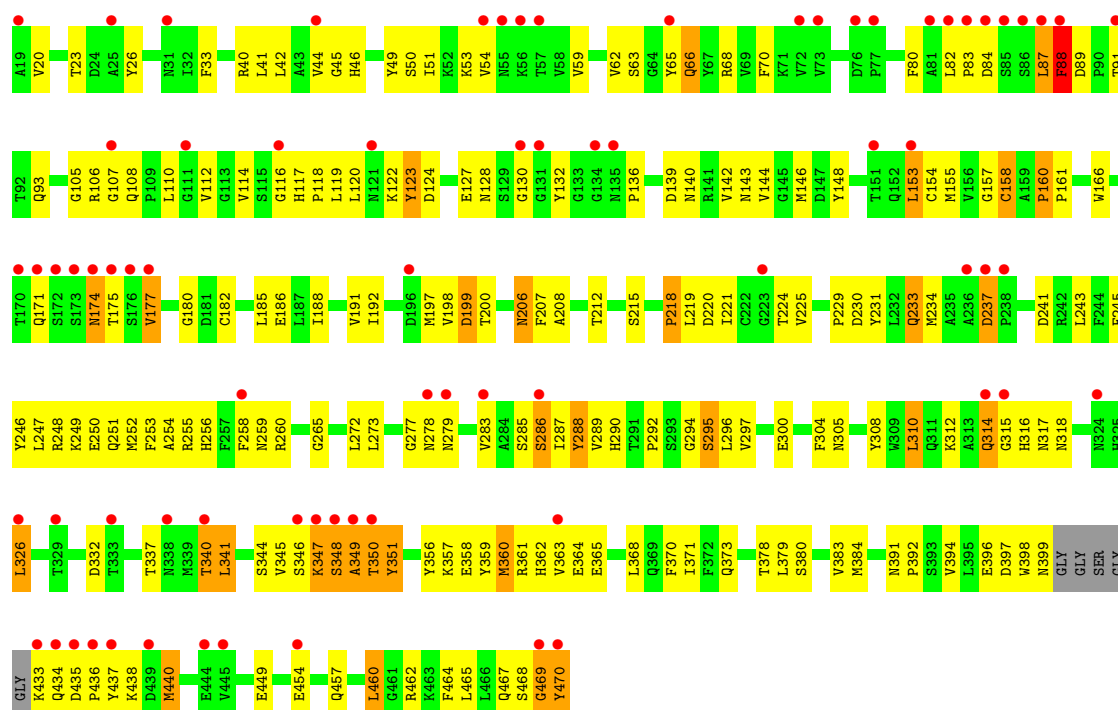


• Molecule 1: Major capsid protein L1





● Molecule 1: Major capsid protein L1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.71Å 159.97Å 158.44Å 90.00° 101.83° 90.00°	Depositor
Resolution (Å)	48.24 – 3.20 48.24 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.24-3.20) 46.3 (48.24-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	19.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.289 , 0.317 0.283 , 0.305	Depositor DCC
R_{free} test set	13242 reflections (9.58%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 13.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	16390	wwPDB-VP
Average B, all atoms (Å ²)	4.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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	0.65	1/3361 (0.0%)	0.95	7/4564 (0.2%)
1	B	0.62	0/3361	0.94	5/4564 (0.1%)
1	C	0.62	0/3361	0.94	6/4564 (0.1%)
1	D	0.65	1/3361 (0.0%)	0.96	9/4564 (0.2%)
1	E	0.64	0/3361	0.95	8/4564 (0.2%)
All	All	0.63	2/16805 (0.0%)	0.95	35/22820 (0.2%)

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	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	TYR	C-O	-8.27	1.15	1.23
1	D	345	VAL	N-CA	-7.39	1.39	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	277	GLY	N-CA-C	9.54	135.80	113.18
1	D	277	GLY	N-CA-C	7.78	131.62	113.18
1	E	278	ASN	N-CA-C	-7.12	95.64	110.80
1	D	88	PHE	N-CA-C	6.80	118.68	107.73
1	D	278	ASN	N-CA-C	-6.63	96.69	110.80
1	A	88	PHE	N-CA-C	6.46	118.13	107.73
1	E	88	PHE	N-CA-C	6.42	118.07	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	PHE	N-CA-C	6.10	117.55	107.73
1	B	288	TYR	N-CA-C	5.79	118.37	110.55
1	E	356	TYR	N-CA-C	5.62	118.38	109.50
1	C	160	PRO	CA-C-N	5.61	125.59	120.03
1	C	160	PRO	C-N-CA	5.61	125.59	120.03
1	A	160	PRO	CA-C-N	5.57	125.54	120.03
1	A	160	PRO	C-N-CA	5.57	125.54	120.03
1	D	160	PRO	CA-C-N	5.50	125.47	120.03
1	D	160	PRO	C-N-CA	5.50	125.47	120.03
1	A	356	TYR	N-CA-C	5.47	118.14	109.50
1	B	278	ASN	CB-CA-C	-5.43	108.72	115.89
1	A	288	TYR	N-CA-C	5.40	117.84	110.55
1	D	345	VAL	CA-C-O	-5.31	115.32	119.46
1	E	288	TYR	N-CA-C	5.30	117.70	110.55
1	C	88	PHE	N-CA-C	5.29	116.25	107.73
1	D	83	PRO	N-CA-C	-5.28	107.26	113.86
1	C	288	TYR	N-CA-C	5.27	117.67	110.55
1	C	58	VAL	CB-CA-C	-5.25	107.24	111.71
1	C	83	PRO	N-CA-C	-5.24	107.31	113.86
1	E	160	PRO	CA-C-N	5.19	125.17	120.03
1	E	160	PRO	C-N-CA	5.19	125.17	120.03
1	A	278	ASN	CB-CA-C	-5.18	109.05	115.89
1	E	158	CYS	N-CA-C	-5.15	106.84	112.72
1	A	148	TYR	N-CA-C	5.12	116.54	110.19
1	D	345	VAL	O-C-N	5.09	127.03	121.78
1	B	160	PRO	CA-C-N	5.07	125.05	120.03
1	B	160	PRO	C-N-CA	5.07	125.05	120.03
1	D	288	TYR	N-CA-C	5.03	117.34	110.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	TYR	Sidechain
1	D	351	TYR	Sidechain

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	3278	0	3163	169	0
1	B	3278	0	3163	176	0
1	C	3278	0	3163	176	0
1	D	3278	0	3163	173	0
1	E	3278	0	3163	167	0
All	All	16390	0	15815	730	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (730) 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:259:ASN:HD21	1:A:285:SER:HB3	1.31	0.96
1:C:259:ASN:HD21	1:C:285:SER:HB3	1.31	0.95
1:D:259:ASN:HD21	1:D:285:SER:HB3	1.31	0.94
1:E:259:ASN:HD21	1:E:285:SER:HB3	1.32	0.93
1:B:259:ASN:HD21	1:B:285:SER:HB3	1.30	0.93
1:A:206:ASN:C	1:A:206:ASN:HD22	1.85	0.83
1:E:206:ASN:C	1:E:206:ASN:HD22	1.87	0.82
1:B:206:ASN:C	1:B:206:ASN:HD22	1.87	0.81
1:A:457:GLN:HE22	1:B:20:VAL:H	1.29	0.80
1:D:206:ASN:C	1:D:206:ASN:HD22	1.86	0.79
1:A:123:TYR:CE1	1:A:136:PRO:HB3	2.20	0.76
1:E:206:ASN:HD21	1:E:208:ALA:HB3	1.50	0.76
1:A:51:ILE:HB	1:A:59:VAL:HB	1.66	0.76
1:E:123:TYR:CE1	1:E:136:PRO:HB3	2.21	0.76
1:C:206:ASN:HD22	1:C:206:ASN:C	1.90	0.75
1:B:206:ASN:HD21	1:B:208:ALA:HB3	1.50	0.75
1:B:51:ILE:HB	1:B:59:VAL:HB	1.69	0.75
1:B:123:TYR:CE1	1:B:136:PRO:HB3	2.21	0.74
1:C:177:VAL:O	1:C:177:VAL:HG23	1.86	0.74
1:D:118:PRO:HD3	1:D:219:LEU:HD21	1.69	0.74
1:D:123:TYR:CE1	1:D:136:PRO:HB3	2.22	0.73
1:E:63:SER:H	1:E:66:GLN:NE2	1.86	0.73
1:E:51:ILE:HB	1:E:59:VAL:HB	1.69	0.73
1:B:118:PRO:HD3	1:B:219:LEU:HD21	1.70	0.72
1:A:20:VAL:H	1:E:457:GLN:HE22	1.38	0.72
1:C:206:ASN:HD21	1:C:208:ALA:HB3	1.54	0.72
1:C:310:LEU:HD23	1:C:310:LEU:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:HD21	1:A:208:ALA:HB3	1.55	0.71
1:C:123:TYR:CE1	1:C:136:PRO:HB3	2.25	0.71
1:A:63:SER:H	1:A:66:GLN:NE2	1.88	0.71
1:D:177:VAL:HG23	1:D:177:VAL:O	1.91	0.71
1:E:118:PRO:HD3	1:E:219:LEU:HD21	1.72	0.71
1:D:63:SER:H	1:D:66:GLN:NE2	1.88	0.71
1:C:363:VAL:HG11	1:D:166:TRP:CZ2	2.25	0.71
1:D:457:GLN:HE22	1:E:20:VAL:H	1.37	0.71
1:A:166:TRP:CZ2	1:E:363:VAL:HG11	2.27	0.70
1:A:346:SER:O	1:A:348:SER:N	2.23	0.70
1:B:177:VAL:HG23	1:B:177:VAL:O	1.91	0.70
1:D:206:ASN:HD21	1:D:208:ALA:HB3	1.56	0.70
1:A:118:PRO:HD3	1:A:219:LEU:HD21	1.74	0.70
1:C:457:GLN:HE22	1:D:20:VAL:H	1.39	0.70
1:D:51:ILE:HB	1:D:59:VAL:HB	1.74	0.70
1:B:435:ASP:OD2	1:B:436:PRO:HD2	1.92	0.70
1:C:118:PRO:HD3	1:C:219:LEU:HD21	1.74	0.69
1:A:344:SER:OG	1:A:347:LYS:HE3	1.92	0.69
1:E:177:VAL:O	1:E:177:VAL:HG23	1.91	0.68
1:E:435:ASP:OD2	1:E:436:PRO:HD2	1.93	0.68
1:C:106:ARG:H	1:C:305:ASN:HD21	1.41	0.68
1:C:63:SER:H	1:C:66:GLN:NE2	1.91	0.68
1:B:63:SER:H	1:B:66:GLN:NE2	1.92	0.68
1:A:177:VAL:HG23	1:A:177:VAL:O	1.93	0.68
1:D:310:LEU:HD23	1:D:310:LEU:H	1.59	0.67
1:C:435:ASP:OD2	1:C:436:PRO:HD2	1.95	0.67
1:A:363:VAL:HG11	1:B:166:TRP:CZ2	2.29	0.67
1:B:310:LEU:H	1:B:310:LEU:HD23	1.59	0.67
1:B:457:GLN:HE22	1:C:20:VAL:H	1.43	0.67
1:A:259:ASN:ND2	1:A:285:SER:HB3	2.08	0.67
1:D:363:VAL:HG11	1:E:166:TRP:CZ2	2.30	0.66
1:C:234:MET:O	1:C:237:ASP:HB2	1.95	0.66
1:A:310:LEU:HD23	1:A:310:LEU:H	1.61	0.66
1:E:106:ARG:H	1:E:305:ASN:HD21	1.42	0.66
1:A:234:MET:O	1:A:237:ASP:HB2	1.96	0.66
1:A:106:ARG:H	1:A:305:ASN:HD21	1.44	0.66
1:C:259:ASN:ND2	1:C:285:SER:HB3	2.10	0.66
1:D:234:MET:O	1:D:237:ASP:HB2	1.96	0.66
1:A:435:ASP:OD2	1:A:436:PRO:HD2	1.96	0.65
1:D:117:HIS:HA	1:D:219:LEU:CD2	2.26	0.65
1:E:310:LEU:H	1:E:310:LEU:HD23	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:H	1:C:252:MET:HE1	1.61	0.65
1:B:234:MET:O	1:B:237:ASP:HB2	1.97	0.65
1:E:44:VAL:HG22	1:E:363:VAL:HG22	1.77	0.65
1:E:259:ASN:ND2	1:E:285:SER:HB3	2.10	0.64
1:C:62:VAL:HA	1:C:66:GLN:HE22	1.63	0.64
1:A:117:HIS:HA	1:A:219:LEU:CD2	2.28	0.64
1:B:300:GLU:OE1	1:C:249:LYS:HE2	1.97	0.64
1:E:117:HIS:HA	1:E:219:LEU:CD2	2.27	0.64
1:C:51:ILE:HB	1:C:59:VAL:HB	1.78	0.64
1:D:435:ASP:OD2	1:D:436:PRO:HD2	1.97	0.64
1:A:62:VAL:HA	1:A:66:GLN:HE22	1.62	0.63
1:A:344:SER:CB	1:B:212:THR:HG21	2.28	0.63
1:B:117:HIS:HA	1:B:219:LEU:CD2	2.28	0.63
1:C:117:HIS:HA	1:C:219:LEU:CD2	2.27	0.63
1:E:259:ASN:HD21	1:E:285:SER:CB	2.09	0.63
1:C:198:VAL:HG12	1:C:199:ASP:O	1.98	0.63
1:D:259:ASN:ND2	1:D:285:SER:HB3	2.10	0.63
1:D:198:VAL:HG12	1:D:199:ASP:O	1.99	0.62
1:A:44:VAL:HG22	1:A:363:VAL:HG22	1.80	0.62
1:B:259:ASN:ND2	1:B:285:SER:HB3	2.09	0.62
1:E:62:VAL:HA	1:E:66:GLN:HE22	1.64	0.62
1:A:259:ASN:HD21	1:A:285:SER:CB	2.07	0.62
1:B:106:ARG:H	1:B:305:ASN:HD21	1.46	0.62
1:A:118:PRO:HG3	1:B:286:SER:HB3	1.82	0.61
1:E:234:MET:O	1:E:237:ASP:HB2	1.98	0.61
1:A:206:ASN:C	1:A:206:ASN:ND2	2.57	0.61
1:E:153:LEU:HD12	1:E:154:CYS:N	2.16	0.61
1:B:82:LEU:HB3	1:B:83:PRO:HD2	1.82	0.61
1:C:44:VAL:HG22	1:C:363:VAL:HG22	1.82	0.61
1:A:234:MET:HB3	1:A:243:LEU:HD22	1.82	0.61
1:A:259:ASN:HD22	1:A:260:ARG:N	1.99	0.61
1:B:259:ASN:HD22	1:B:260:ARG:N	1.99	0.61
1:D:62:VAL:HA	1:D:66:GLN:HE22	1.65	0.61
1:D:259:ASN:HD21	1:D:285:SER:CB	2.09	0.61
1:A:198:VAL:HG12	1:A:199:ASP:O	2.00	0.61
1:D:153:LEU:HD12	1:D:154:CYS:N	2.16	0.61
1:B:234:MET:HB3	1:B:243:LEU:HD22	1.82	0.61
1:B:259:ASN:HD21	1:B:285:SER:CB	2.09	0.60
1:E:198:VAL:HG12	1:E:199:ASP:O	2.01	0.60
1:A:120:LEU:HD23	1:A:144:VAL:HG21	1.81	0.60
1:C:259:ASN:HD22	1:C:260:ARG:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:LEU:N	1:E:341:LEU:HD23	2.16	0.60
1:A:344:SER:HB3	1:B:212:THR:HG21	1.82	0.60
1:C:40:ARG:O	1:C:41:LEU:HD23	2.02	0.60
1:B:62:VAL:HA	1:B:66:GLN:HE22	1.66	0.60
1:A:148:TYR:OH	1:A:218:PRO:HB2	2.02	0.59
1:D:88:PHE:HB2	1:D:93:GLN:OE1	2.02	0.59
1:E:252:MET:HG2	1:E:253:PHE:N	2.18	0.59
1:B:33:PHE:CE2	1:B:373:GLN:HB2	2.36	0.59
1:B:198:VAL:HG12	1:B:199:ASP:O	2.02	0.59
1:B:148:TYR:OH	1:B:218:PRO:HB2	2.03	0.59
1:B:171:GLN:OE1	1:B:177:VAL:HG11	2.03	0.59
1:D:345:VAL:HG22	1:E:180:GLY:HA3	1.83	0.59
1:E:259:ASN:HD22	1:E:260:ARG:N	2.01	0.59
1:A:166:TRP:HZ2	1:E:363:VAL:HG11	1.65	0.59
1:D:106:ARG:H	1:D:305:ASN:HD21	1.48	0.59
1:B:120:LEU:HD23	1:B:144:VAL:HG21	1.85	0.59
1:A:112:VAL:H	1:B:252:MET:HE1	1.67	0.58
1:A:33:PHE:CE2	1:A:373:GLN:HB2	2.37	0.58
1:A:312:LYS:HA	1:A:318:ASN:HD21	1.68	0.58
1:C:234:MET:HB3	1:C:243:LEU:HD22	1.84	0.58
1:E:107:GLY:HA3	1:E:365:GLU:CD	2.28	0.58
1:A:286:SER:HB3	1:E:118:PRO:HG3	1.85	0.58
1:B:346:SER:O	1:B:348:SER:N	2.36	0.58
1:C:153:LEU:HA	1:C:247:LEU:O	2.03	0.58
1:D:234:MET:HB3	1:D:243:LEU:HD22	1.85	0.58
1:B:363:VAL:HG11	1:C:166:TRP:CZ2	2.37	0.58
1:D:259:ASN:HD22	1:D:260:ARG:N	2.02	0.58
1:B:345:VAL:HG22	1:C:180:GLY:HA3	1.86	0.58
1:C:112:VAL:H	1:D:252:MET:HE1	1.67	0.58
1:B:82:LEU:HB2	1:B:84:ASP:O	2.03	0.58
1:D:82:LEU:HB3	1:D:83:PRO:HD2	1.86	0.58
1:E:82:LEU:HB3	1:E:83:PRO:HD2	1.85	0.58
1:B:40:ARG:O	1:B:41:LEU:HD23	2.03	0.58
1:B:44:VAL:HG22	1:B:363:VAL:HG22	1.84	0.58
1:A:153:LEU:HD12	1:A:154:CYS:N	2.20	0.57
1:A:153:LEU:HA	1:A:247:LEU:O	2.05	0.57
1:B:344:SER:HB3	1:C:212:THR:HG21	1.85	0.57
1:B:107:GLY:HA3	1:B:365:GLU:CD	2.29	0.57
1:D:33:PHE:CE2	1:D:373:GLN:HB2	2.40	0.57
1:A:249:LYS:HE2	1:E:300:GLU:OE1	2.05	0.57
1:A:252:MET:HE1	1:E:112:VAL:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:HG11	1:B:166:TRP:HZ2	1.67	0.57
1:C:289:VAL:HG12	1:C:290:HIS:N	2.18	0.57
1:C:107:GLY:HA3	1:C:365:GLU:CD	2.30	0.57
1:A:82:LEU:HB3	1:A:83:PRO:HD2	1.87	0.57
1:A:252:MET:HG2	1:A:253:PHE:N	2.18	0.57
1:C:171:GLN:OE1	1:C:177:VAL:HG11	2.04	0.57
1:D:40:ARG:O	1:D:41:LEU:HD23	2.05	0.57
1:D:44:VAL:HG22	1:D:363:VAL:HG22	1.87	0.57
1:D:279:ASN:OD1	1:D:280:ARG:NH1	2.37	0.57
1:C:312:LYS:HA	1:C:318:ASN:HD21	1.70	0.56
1:E:234:MET:HB3	1:E:243:LEU:HD22	1.87	0.56
1:C:82:LEU:HB3	1:C:83:PRO:HD2	1.87	0.56
1:D:341:LEU:N	1:D:341:LEU:HD23	2.20	0.56
1:B:312:LYS:HA	1:B:318:ASN:HD21	1.70	0.56
1:E:148:TYR:OH	1:E:218:PRO:HB2	2.04	0.56
1:A:127:GLU:OE1	1:E:256:HIS:HE1	1.89	0.56
1:E:346:SER:O	1:E:348:SER:N	2.39	0.56
1:A:341:LEU:HD23	1:A:341:LEU:N	2.21	0.56
1:A:344:SER:OG	1:B:212:THR:HG21	2.06	0.56
1:A:345:VAL:HG12	1:A:345:VAL:O	2.05	0.56
1:C:344:SER:CB	1:D:212:THR:HG21	2.35	0.56
1:D:344:SER:OG	1:D:347:LYS:HG3	2.06	0.56
1:B:341:LEU:N	1:B:341:LEU:HD23	2.21	0.56
1:E:33:PHE:CE2	1:E:373:GLN:HB2	2.41	0.56
1:C:344:SER:HB3	1:D:212:THR:HG21	1.88	0.55
1:D:107:GLY:HA3	1:D:365:GLU:CD	2.31	0.55
1:D:346:SER:O	1:D:348:SER:N	2.38	0.55
1:C:148:TYR:OH	1:C:218:PRO:HB2	2.04	0.55
1:B:153:LEU:HA	1:B:247:LEU:O	2.05	0.55
1:C:120:LEU:HD23	1:C:144:VAL:HG21	1.87	0.55
1:B:362:HIS:CD2	1:B:363:VAL:H	2.24	0.55
1:E:158:CYS:SG	1:E:241:ASP:HB3	2.46	0.55
1:C:363:VAL:HG11	1:D:166:TRP:HZ2	1.68	0.55
1:A:171:GLN:OE1	1:A:177:VAL:HG11	2.07	0.55
1:C:33:PHE:CE2	1:C:373:GLN:HB2	2.40	0.55
1:C:153:LEU:HD12	1:C:154:CYS:N	2.21	0.55
1:D:23:THR:CG2	1:D:317:ASN:HA	2.36	0.55
1:B:256:HIS:HE1	1:C:127:GLU:OE1	1.89	0.55
1:C:312:LYS:HD2	1:C:318:ASN:HD21	1.72	0.55
1:A:251:GLN:HB2	1:E:296:LEU:HD12	1.88	0.55
1:B:435:ASP:HB3	1:B:438:LYS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ASN:HD21	1:C:285:SER:CB	2.11	0.55
1:D:153:LEU:HA	1:D:247:LEU:O	2.07	0.55
1:D:362:HIS:CD2	1:D:363:VAL:H	2.25	0.55
1:A:40:ARG:O	1:A:41:LEU:HD23	2.06	0.54
1:C:82:LEU:HB2	1:C:84:ASP:O	2.07	0.54
1:C:346:SER:O	1:C:348:SER:N	2.40	0.54
1:D:148:TYR:OH	1:D:218:PRO:HB2	2.06	0.54
1:E:153:LEU:HA	1:E:247:LEU:O	2.07	0.54
1:A:256:HIS:HE1	1:B:127:GLU:OE1	1.90	0.54
1:D:363:VAL:HG11	1:E:166:TRP:HZ2	1.72	0.54
1:E:289:VAL:HG12	1:E:290:HIS:N	2.22	0.54
1:D:312:LYS:HD2	1:D:318:ASN:HD21	1.72	0.54
1:B:252:MET:HG2	1:B:253:PHE:N	2.21	0.54
1:D:312:LYS:HA	1:D:318:ASN:HD21	1.71	0.54
1:D:252:MET:HG2	1:D:253:PHE:N	2.22	0.54
1:B:289:VAL:HG12	1:B:290:HIS:N	2.22	0.54
1:D:158:CYS:SG	1:D:241:ASP:HB3	2.47	0.54
1:C:357:LYS:HG2	1:D:263:THR:OG1	2.08	0.54
1:C:435:ASP:HB3	1:C:438:LYS:HB2	1.90	0.54
1:D:300:GLU:OE1	1:E:249:LYS:HE2	2.06	0.54
1:A:362:HIS:CD2	1:A:363:VAL:H	2.26	0.54
1:C:341:LEU:HD23	1:C:341:LEU:N	2.22	0.54
1:D:112:VAL:H	1:E:252:MET:HE1	1.72	0.54
1:B:344:SER:CB	1:C:212:THR:HG21	2.38	0.53
1:D:120:LEU:HD23	1:D:144:VAL:HG21	1.89	0.53
1:E:312:LYS:HA	1:E:318:ASN:HD21	1.72	0.53
1:C:434:GLN:HE21	1:C:435:ASP:H	1.55	0.53
1:E:82:LEU:HB2	1:E:84:ASP:O	2.09	0.53
1:A:107:GLY:HA3	1:A:365:GLU:CD	2.33	0.53
1:C:88:PHE:HB2	1:C:93:GLN:OE1	2.08	0.53
1:C:119:LEU:O	1:C:215:SER:HB3	2.08	0.53
1:D:314:GLN:OE1	1:D:315:GLY:N	2.42	0.53
1:A:435:ASP:HB3	1:A:438:LYS:HB2	1.89	0.53
1:B:158:CYS:SG	1:B:241:ASP:HB3	2.48	0.53
1:C:158:CYS:SG	1:C:241:ASP:HB3	2.48	0.53
1:E:40:ARG:O	1:E:41:LEU:HD23	2.07	0.53
1:D:468:SER:O	1:D:470:TYR:N	2.36	0.53
1:E:344:SER:OG	1:E:347:LYS:HE3	2.08	0.53
1:D:345:VAL:HG22	1:E:180:GLY:CA	2.38	0.53
1:E:23:THR:CG2	1:E:317:ASN:HA	2.39	0.53
1:E:105:GLY:HA2	1:E:305:ASN:ND2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HB2	1:A:84:ASP:O	2.09	0.53
1:A:296:LEU:HD12	1:B:251:GLN:HB2	1.91	0.53
1:B:153:LEU:HD12	1:B:154:CYS:N	2.24	0.53
1:C:344:SER:OG	1:C:347:LYS:HG3	2.08	0.53
1:B:110:LEU:HD22	1:C:250:GLU:HG3	1.91	0.53
1:B:119:LEU:O	1:B:215:SER:HB3	2.09	0.53
1:B:234:MET:HB3	1:B:243:LEU:CD2	2.39	0.53
1:C:23:THR:CG2	1:C:317:ASN:HA	2.39	0.53
1:C:362:HIS:CD2	1:C:363:VAL:H	2.26	0.53
1:E:186:GLU:HG2	1:E:188:ILE:HD12	1.91	0.53
1:E:341:LEU:HD23	1:E:341:LEU:H	1.73	0.53
1:E:148:TYR:CG	1:E:200:THR:HB	2.44	0.52
1:A:207:PHE:CE1	1:A:221:ILE:HD12	2.44	0.52
1:B:312:LYS:HD2	1:B:318:ASN:HD21	1.74	0.52
1:B:186:GLU:HG2	1:B:188:ILE:HD12	1.91	0.52
1:C:45:GLY:O	1:C:361:ARG:HD3	2.09	0.52
1:D:23:THR:HG21	1:D:317:ASN:HA	1.92	0.52
1:D:371:ILE:HG13	1:D:460:LEU:HD13	1.91	0.52
1:A:250:GLU:HG3	1:E:110:LEU:HD22	1.90	0.52
1:C:105:GLY:HA2	1:C:305:ASN:ND2	2.24	0.52
1:C:206:ASN:C	1:C:206:ASN:ND2	2.61	0.52
1:A:234:MET:HB3	1:A:243:LEU:CD2	2.39	0.52
1:B:93:GLN:NE2	1:B:378:THR:HG22	2.25	0.52
1:B:112:VAL:N	1:C:252:MET:HE1	2.24	0.52
1:C:177:VAL:O	1:C:177:VAL:CG2	2.57	0.52
1:D:171:GLN:OE1	1:D:177:VAL:HG11	2.09	0.52
1:D:255:ARG:NH1	1:E:127:GLU:OE1	2.41	0.52
1:A:300:GLU:OE1	1:B:249:LYS:HE2	2.09	0.52
1:B:344:SER:OG	1:B:347:LYS:HG3	2.09	0.52
1:B:380:SER:OG	1:B:383:VAL:HG23	2.10	0.52
1:D:82:LEU:HB2	1:D:84:ASP:O	2.09	0.52
1:D:207:PHE:CE1	1:D:221:ILE:HD12	2.45	0.52
1:D:344:SER:HB3	1:E:212:THR:HG21	1.92	0.52
1:A:186:GLU:HG2	1:A:188:ILE:HD12	1.92	0.52
1:B:88:PHE:HB2	1:B:93:GLN:OE1	2.10	0.52
1:D:45:GLY:O	1:D:361:ARG:HD3	2.09	0.52
1:D:289:VAL:HG12	1:D:290:HIS:N	2.25	0.52
1:E:362:HIS:CD2	1:E:363:VAL:H	2.28	0.52
1:D:119:LEU:O	1:D:215:SER:HB3	2.10	0.52
1:E:371:ILE:CD1	1:E:464:PHE:HB2	2.40	0.52
1:C:252:MET:HG2	1:C:253:PHE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:ASP:HB3	1:E:438:LYS:HB2	1.91	0.51
1:E:119:LEU:O	1:E:215:SER:HB3	2.10	0.51
1:B:437:TYR:HB3	1:B:440:MET:HG3	1.92	0.51
1:D:118:PRO:HG3	1:E:286:SER:HB3	1.91	0.51
1:E:88:PHE:HB2	1:E:93:GLN:OE1	2.11	0.51
1:E:207:PHE:CE1	1:E:221:ILE:HD12	2.46	0.51
1:A:342:CYS:SG	1:B:213:ASN:ND2	2.83	0.51
1:B:207:PHE:CE1	1:B:221:ILE:HD12	2.45	0.51
1:B:118:PRO:HG3	1:C:286:SER:HB3	1.93	0.51
1:E:118:PRO:CD	1:E:219:LEU:HD21	2.40	0.51
1:C:148:TYR:CG	1:C:200:THR:HB	2.46	0.51
1:B:105:GLY:HA2	1:B:305:ASN:ND2	2.26	0.50
1:B:371:ILE:HG13	1:B:460:LEU:HD13	1.93	0.50
1:E:341:LEU:N	1:E:341:LEU:CD2	2.74	0.50
1:B:206:ASN:C	1:B:206:ASN:ND2	2.59	0.50
1:B:371:ILE:CD1	1:B:464:PHE:HB2	2.42	0.50
1:C:207:PHE:CE1	1:C:221:ILE:HD12	2.46	0.50
1:C:371:ILE:HG13	1:C:460:LEU:HD13	1.93	0.50
1:A:289:VAL:HG12	1:A:290:HIS:N	2.26	0.50
1:A:371:ILE:CD1	1:A:464:PHE:HB2	2.41	0.50
1:B:341:LEU:HD23	1:B:341:LEU:H	1.76	0.50
1:C:50:SER:C	1:C:51:ILE:HD12	2.35	0.50
1:A:105:GLY:HA2	1:A:305:ASN:ND2	2.27	0.50
1:A:347:LYS:HE3	1:B:212:THR:CG2	2.42	0.50
1:B:468:SER:O	1:B:470:TYR:N	2.41	0.50
1:C:380:SER:OG	1:C:383:VAL:HG23	2.11	0.50
1:D:105:GLY:HA2	1:D:305:ASN:ND2	2.26	0.50
1:C:361:ARG:NH1	1:D:182:CYS:SG	2.85	0.50
1:A:148:TYR:CG	1:A:200:THR:HB	2.45	0.50
1:A:380:SER:OG	1:A:383:VAL:HG23	2.12	0.50
1:D:341:LEU:HD23	1:D:341:LEU:H	1.76	0.50
1:E:434:GLN:HE21	1:E:435:ASP:H	1.58	0.50
1:A:40:ARG:HG2	1:A:42:LEU:HD13	1.93	0.50
1:A:180:GLY:HA3	1:E:345:VAL:HG22	1.94	0.50
1:A:341:LEU:HD23	1:A:341:LEU:H	1.77	0.50
1:B:157:GLY:O	1:B:326:LEU:HD23	2.12	0.50
1:C:166:TRP:HB3	1:C:185:LEU:HD12	1.93	0.50
1:D:118:PRO:CD	1:D:219:LEU:HD21	2.39	0.50
1:C:118:PRO:HG3	1:D:286:SER:HB3	1.92	0.50
1:D:437:TYR:HB3	1:D:440:MET:HG3	1.94	0.50
1:E:171:GLN:OE1	1:E:177:VAL:HG11	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD22	1:B:250:GLU:HG3	1.93	0.49
1:D:380:SER:OG	1:D:383:VAL:HG23	2.12	0.49
1:E:230:ASP:CG	1:E:233:GLN:HB3	2.37	0.49
1:A:45:GLY:O	1:A:361:ARG:HD3	2.12	0.49
1:B:363:VAL:HG11	1:C:166:TRP:HZ2	1.75	0.49
1:C:359:TYR:CE2	1:D:265:GLY:HA3	2.46	0.49
1:E:120:LEU:HD23	1:E:144:VAL:HG21	1.94	0.49
1:A:119:LEU:O	1:A:215:SER:HB3	2.12	0.49
1:D:434:GLN:HE21	1:D:435:ASP:H	1.59	0.49
1:E:166:TRP:HB3	1:E:185:LEU:HD12	1.94	0.49
1:E:312:LYS:HD2	1:E:318:ASN:HD21	1.77	0.49
1:E:468:SER:O	1:E:470:TYR:N	2.40	0.49
1:A:23:THR:CG2	1:A:317:ASN:HA	2.42	0.49
1:C:259:ASN:ND2	1:C:259:ASN:C	2.71	0.49
1:D:197:MET:HE2	1:D:220:ASP:O	2.12	0.49
1:E:206:ASN:C	1:E:206:ASN:ND2	2.58	0.49
1:B:314:GLN:OE1	1:B:315:GLY:N	2.45	0.49
1:C:51:ILE:HG22	1:C:51:ILE:O	2.12	0.49
1:E:348:SER:O	1:E:349:ALA:C	2.56	0.49
1:C:40:ARG:HG2	1:C:42:LEU:HD13	1.94	0.49
1:C:256:HIS:HE1	1:D:127:GLU:OE1	1.95	0.49
1:D:256:HIS:HE1	1:E:127:GLU:OE1	1.96	0.49
1:E:345:VAL:HG12	1:E:345:VAL:O	2.13	0.49
1:A:348:SER:O	1:A:349:ALA:C	2.56	0.49
1:C:23:THR:HG21	1:C:317:ASN:HA	1.94	0.49
1:D:89:ASP:C	1:D:91:THR:H	2.20	0.49
1:A:93:GLN:HB3	1:A:378:THR:HA	1.95	0.49
1:A:437:TYR:HB3	1:A:440:MET:HG3	1.94	0.49
1:B:350:THR:O	1:B:351:TYR:C	2.55	0.49
1:C:234:MET:HB3	1:C:243:LEU:CD2	2.43	0.49
1:D:186:GLU:HG2	1:D:188:ILE:HD12	1.95	0.49
1:D:344:SER:CB	1:E:212:THR:HG21	2.43	0.49
1:E:45:GLY:O	1:E:361:ARG:HD3	2.13	0.49
1:A:93:GLN:NE2	1:A:378:THR:HG22	2.28	0.49
1:B:344:SER:OG	1:B:347:LYS:HE3	2.13	0.49
1:C:434:GLN:NE2	1:C:435:ASP:H	2.10	0.49
1:D:93:GLN:HB3	1:D:378:THR:HA	1.95	0.49
1:D:166:TRP:HB3	1:D:185:LEU:HD12	1.94	0.49
1:D:312:LYS:HD2	1:D:318:ASN:ND2	2.28	0.49
1:A:371:ILE:HG13	1:A:460:LEU:HD13	1.94	0.48
1:C:312:LYS:HD2	1:C:318:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:VAL:HG12	1:C:345:VAL:O	2.12	0.48
1:D:206:ASN:C	1:D:206:ASN:ND2	2.57	0.48
1:A:23:THR:HG21	1:A:317:ASN:HA	1.95	0.48
1:A:118:PRO:CD	1:A:219:LEU:HD21	2.41	0.48
1:A:462:ARG:NH1	1:B:315:GLY:HA2	2.27	0.48
1:C:93:GLN:HB3	1:C:378:THR:HA	1.95	0.48
1:C:118:PRO:CD	1:C:219:LEU:HD21	2.41	0.48
1:C:230:ASP:CG	1:C:233:GLN:HB3	2.38	0.48
1:D:146:MET:HE2	1:D:292:PRO:HD2	1.95	0.48
1:E:65:TYR:CE2	1:E:148:TYR:HB2	2.48	0.48
1:A:109:PRO:HB3	1:B:228:TYR:CD1	2.48	0.48
1:A:259:ASN:HD22	1:A:259:ASN:C	2.22	0.48
1:C:344:SER:OG	1:D:212:THR:HG21	2.14	0.48
1:D:234:MET:HB3	1:D:243:LEU:CD2	2.44	0.48
1:E:360:MET:HE2	1:E:360:MET:HA	1.95	0.48
1:C:437:TYR:HB3	1:C:440:MET:HG3	1.95	0.48
1:E:23:THR:HG21	1:E:317:ASN:HA	1.95	0.48
1:A:146:MET:HE2	1:A:292:PRO:HD2	1.96	0.48
1:A:391:ASN:CG	1:A:394:VAL:HG23	2.39	0.48
1:B:89:ASP:C	1:B:91:THR:H	2.21	0.48
1:E:160:PRO:HB2	1:E:191:VAL:HG13	1.95	0.48
1:A:246:TYR:CD1	1:A:246:TYR:C	2.92	0.48
1:A:468:SER:O	1:A:470:TYR:N	2.41	0.48
1:B:312:LYS:HD2	1:B:318:ASN:ND2	2.28	0.48
1:A:166:TRP:HB3	1:A:185:LEU:HD12	1.96	0.48
1:B:397:ASP:O	1:B:399:ASN:N	2.47	0.48
1:D:148:TYR:CG	1:D:200:THR:HB	2.47	0.48
1:E:371:ILE:HG13	1:E:460:LEU:HD13	1.96	0.48
1:B:345:VAL:HG12	1:B:345:VAL:O	2.12	0.48
1:C:146:MET:HE2	1:C:292:PRO:HD2	1.96	0.48
1:D:345:VAL:HG12	1:D:345:VAL:O	2.14	0.48
1:B:146:MET:HE2	1:B:292:PRO:HD2	1.96	0.48
1:B:148:TYR:CG	1:B:200:THR:HB	2.48	0.48
1:E:234:MET:HB3	1:E:243:LEU:CD2	2.44	0.48
1:B:93:GLN:HB3	1:B:378:THR:HA	1.96	0.47
1:B:341:LEU:N	1:B:341:LEU:CD2	2.77	0.47
1:C:300:GLU:OE1	1:D:249:LYS:HE2	2.14	0.47
1:D:435:ASP:HB3	1:D:438:LYS:HB2	1.95	0.47
1:D:391:ASN:CG	1:D:394:VAL:HG23	2.38	0.47
1:B:65:TYR:CE2	1:B:148:TYR:HB2	2.49	0.47
1:D:340:THR:OG1	1:D:360:MET:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HG2	1:B:42:LEU:HD13	1.97	0.47
1:B:118:PRO:CD	1:B:219:LEU:HD21	2.40	0.47
1:E:87:LEU:O	1:E:88:PHE:HB3	2.14	0.47
1:A:341:LEU:N	1:A:341:LEU:CD2	2.78	0.47
1:C:65:TYR:CE2	1:C:148:TYR:HB2	2.48	0.47
1:C:89:ASP:C	1:C:91:THR:H	2.21	0.47
1:C:161:PRO:HG2	1:C:192:ILE:HB	1.96	0.47
1:C:314:GLN:OE1	1:C:315:GLY:N	2.48	0.47
1:D:341:LEU:N	1:D:341:LEU:CD2	2.77	0.47
1:E:93:GLN:HB3	1:E:378:THR:HA	1.96	0.47
1:E:350:THR:O	1:E:351:TYR:C	2.57	0.47
1:B:379:LEU:HB3	1:B:384:MET:HE1	1.97	0.47
1:C:344:SER:OG	1:C:347:LYS:HE3	2.14	0.47
1:D:161:PRO:HG2	1:D:192:ILE:HB	1.96	0.47
1:E:89:ASP:C	1:E:91:THR:H	2.22	0.47
1:A:112:VAL:N	1:B:252:MET:HE1	2.30	0.47
1:A:160:PRO:HB2	1:A:191:VAL:HG13	1.96	0.47
1:A:229:PRO:HB2	1:A:231:TYR:CE1	2.49	0.47
1:A:312:LYS:HD2	1:A:318:ASN:HD21	1.80	0.47
1:A:462:ARG:HH11	1:B:315:GLY:HA2	1.79	0.47
1:B:174:ASN:O	1:B:175:THR:C	2.58	0.47
1:D:371:ILE:CD1	1:D:464:PHE:HB2	2.44	0.47
1:E:146:MET:HE2	1:E:292:PRO:HD2	1.97	0.47
1:E:392:PRO:O	1:E:396:GLU:HG3	2.15	0.47
1:A:23:THR:HA	1:A:26:TYR:CE2	2.49	0.47
1:A:197:MET:HE2	1:A:220:ASP:O	2.14	0.47
1:A:230:ASP:CG	1:A:233:GLN:HB3	2.40	0.47
1:C:468:SER:O	1:C:470:TYR:N	2.38	0.47
1:A:287:ILE:HD12	1:E:358:GLU:HB2	1.97	0.47
1:B:23:THR:CG2	1:B:317:ASN:HA	2.45	0.47
1:C:371:ILE:CD1	1:C:464:PHE:HB2	2.44	0.47
1:B:229:PRO:HB2	1:B:231:TYR:CE1	2.50	0.46
1:B:464:PHE:O	1:B:465:LEU:C	2.57	0.46
1:D:54:VAL:HG12	1:D:54:VAL:O	2.15	0.46
1:E:157:GLY:O	1:E:326:LEU:HD23	2.15	0.46
1:A:89:ASP:C	1:A:91:THR:H	2.22	0.46
1:A:457:GLN:NE2	1:B:20:VAL:H	2.04	0.46
1:C:87:LEU:O	1:C:88:PHE:HB3	2.15	0.46
1:C:457:GLN:NE2	1:D:20:VAL:H	2.11	0.46
1:D:111:GLY:HA2	1:E:252:MET:HE1	1.97	0.46
1:E:259:ASN:HD22	1:E:259:ASN:C	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:TYR:CD2	1:B:182:CYS:HB2	2.51	0.46
1:C:23:THR:HA	1:C:26:TYR:CE2	2.51	0.46
1:C:112:VAL:N	1:D:252:MET:HE1	2.30	0.46
1:D:40:ARG:HG2	1:D:42:LEU:HD13	1.98	0.46
1:A:87:LEU:O	1:A:88:PHE:HB3	2.14	0.46
1:D:112:VAL:N	1:E:252:MET:HE1	2.30	0.46
1:E:68:ARG:HD3	1:E:68:ARG:HA	1.75	0.46
1:A:88:PHE:HB2	1:A:93:GLN:OE1	2.16	0.46
1:A:158:CYS:SG	1:A:241:ASP:HB3	2.55	0.46
1:A:212:THR:HG21	1:E:344:SER:HB3	1.98	0.46
1:C:341:LEU:HD23	1:C:341:LEU:H	1.80	0.46
1:D:116:GLY:HA3	1:E:288:TYR:CE1	2.51	0.46
1:D:160:PRO:HB2	1:D:191:VAL:HG13	1.98	0.46
1:D:230:ASP:CG	1:D:233:GLN:HB3	2.40	0.46
1:E:229:PRO:HB2	1:E:231:TYR:CE1	2.50	0.46
1:A:315:GLY:HA2	1:E:462:ARG:HH11	1.81	0.46
1:B:160:PRO:HB2	1:B:191:VAL:HG13	1.98	0.46
1:C:154:CYS:O	1:C:246:TYR:HA	2.16	0.46
1:D:23:THR:HA	1:D:26:TYR:CE2	2.50	0.46
1:A:350:THR:O	1:A:351:TYR:C	2.58	0.46
1:A:379:LEU:HB3	1:A:384:MET:HE1	1.98	0.46
1:C:106:ARG:H	1:C:305:ASN:ND2	2.11	0.46
1:D:68:ARG:HA	1:D:68:ARG:HD3	1.73	0.46
1:D:229:PRO:HB2	1:D:231:TYR:CE1	2.51	0.46
1:E:391:ASN:CG	1:E:394:VAL:HG23	2.41	0.46
1:A:315:GLY:HA2	1:E:462:ARG:NH1	2.30	0.46
1:E:434:GLN:NE2	1:E:435:ASP:H	2.12	0.46
1:A:347:LYS:HE3	1:B:212:THR:HG21	1.98	0.46
1:A:342:CYS:HB3	1:A:358:GLU:OE1	2.16	0.46
1:C:259:ASN:HD22	1:C:259:ASN:C	2.22	0.46
1:A:65:TYR:CE2	1:A:148:TYR:HB2	2.52	0.45
1:A:434:GLN:HE21	1:A:435:ASP:H	1.64	0.45
1:A:467:GLN:C	1:A:469:GLY:H	2.24	0.45
1:B:88:PHE:HD1	1:B:93:GLN:HG3	1.80	0.45
1:C:341:LEU:N	1:C:341:LEU:CD2	2.79	0.45
1:E:344:SER:OG	1:E:347:LYS:HG3	2.16	0.45
1:A:259:ASN:ND2	1:A:259:ASN:C	2.73	0.45
1:B:166:TRP:HB3	1:B:185:LEU:HD12	1.97	0.45
1:B:259:ASN:HD22	1:B:259:ASN:C	2.23	0.45
1:C:350:THR:O	1:C:351:TYR:C	2.59	0.45
1:E:155:MET:HE1	1:E:229:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:GLN:OE1	1:E:315:GLY:N	2.49	0.45
1:B:50:SER:C	1:B:51:ILE:HD12	2.41	0.45
1:D:65:TYR:CE2	1:D:148:TYR:HB2	2.51	0.45
1:D:110:LEU:HD22	1:E:250:GLU:HG3	1.98	0.45
1:A:54:VAL:HG12	1:A:54:VAL:O	2.17	0.45
1:B:294:GLY:O	1:B:295:SER:O	2.35	0.45
1:B:462:ARG:NH1	1:C:315:GLY:HA2	2.31	0.45
1:C:342:CYS:SG	1:D:213:ASN:ND2	2.89	0.45
1:D:359:TYR:CE2	1:E:265:GLY:HA3	2.51	0.45
1:D:434:GLN:NE2	1:D:435:ASP:H	2.13	0.45
1:E:40:ARG:HG2	1:E:42:LEU:HD13	1.97	0.45
1:E:243:LEU:HG	1:E:243:LEU:O	2.16	0.45
1:C:277:GLY:O	1:C:278:ASN:HB2	2.16	0.45
1:D:350:THR:O	1:D:351:TYR:C	2.59	0.45
1:E:122:LYS:HE3	1:E:258:PHE:CE2	2.51	0.45
1:E:312:LYS:HD2	1:E:318:ASN:ND2	2.32	0.45
1:B:45:GLY:O	1:B:361:ARG:HD3	2.16	0.45
1:C:66:GLN:NE2	1:C:68:ARG:NH2	2.65	0.45
1:D:370:PHE:CD1	1:D:370:PHE:N	2.84	0.45
1:E:224:THR:HB	1:E:225:VAL:H	1.61	0.45
1:B:114:VAL:CG2	1:C:290:HIS:HB3	2.47	0.45
1:C:110:LEU:HD22	1:D:250:GLU:HG3	1.99	0.45
1:C:464:PHE:O	1:C:465:LEU:C	2.60	0.45
1:D:50:SER:C	1:D:51:ILE:HD12	2.41	0.45
1:D:344:SER:OG	1:D:347:LYS:HE3	2.16	0.45
1:A:312:LYS:HD2	1:A:318:ASN:ND2	2.32	0.45
1:A:370:PHE:CD1	1:A:370:PHE:N	2.84	0.45
1:C:23:THR:HG23	1:C:316:HIS:O	2.17	0.45
1:E:197:MET:HE2	1:E:220:ASP:O	2.17	0.45
1:B:111:GLY:HA2	1:C:252:MET:HE1	1.98	0.45
1:C:122:LYS:HE3	1:C:258:PHE:CE2	2.52	0.45
1:D:379:LEU:HB3	1:D:384:MET:HE1	1.98	0.45
1:B:230:ASP:CG	1:B:233:GLN:HB3	2.42	0.45
1:B:245:PHE:CZ	1:B:308:TYR:HB3	2.52	0.45
1:A:182:CYS:HB2	1:E:359:TYR:CD2	2.53	0.44
1:B:197:MET:HE2	1:B:220:ASP:O	2.17	0.44
1:C:347:LYS:HE3	1:D:212:THR:CG2	2.47	0.44
1:A:391:ASN:OD1	1:A:394:VAL:HG23	2.17	0.44
1:D:464:PHE:O	1:D:465:LEU:C	2.59	0.44
1:E:93:GLN:NE2	1:E:378:THR:HG22	2.32	0.44
1:E:259:ASN:ND2	1:E:259:ASN:C	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:MET:HA	1:A:360:MET:HE2	1.99	0.44
1:C:51:ILE:HG12	1:D:266:GLU:CD	2.42	0.44
1:A:68:ARG:HA	1:A:68:ARG:HD3	1.73	0.44
1:A:88:PHE:HD1	1:A:93:GLN:HG3	1.82	0.44
1:A:252:MET:HE1	1:E:112:VAL:N	2.31	0.44
1:A:344:SER:OG	1:A:347:LYS:HG3	2.18	0.44
1:A:358:GLU:HB2	1:B:287:ILE:HD12	2.00	0.44
1:C:188:ILE:HD12	1:C:188:ILE:N	2.33	0.44
1:E:310:LEU:HD23	1:E:310:LEU:N	2.31	0.44
1:B:177:VAL:O	1:B:177:VAL:CG2	2.62	0.44
1:C:246:TYR:CD1	1:C:246:TYR:C	2.94	0.44
1:E:23:THR:HA	1:E:26:TYR:CE2	2.52	0.44
1:A:174:ASN:O	1:A:175:THR:C	2.60	0.44
1:C:255:ARG:NH1	1:D:127:GLU:OE1	2.51	0.44
1:A:157:GLY:O	1:A:326:LEU:HD23	2.17	0.44
1:A:352:THR:HB	1:A:355:ASP:OD1	2.18	0.44
1:B:376:SER:C	1:B:377:ILE:HG13	2.43	0.44
1:B:434:GLN:HE21	1:B:435:ASP:H	1.65	0.44
1:A:122:LYS:HG3	1:A:258:PHE:CD1	2.53	0.44
1:A:251:GLN:HA	1:E:297:VAL:O	2.17	0.44
1:B:154:CYS:O	1:B:246:TYR:HA	2.18	0.44
1:D:359:TYR:CD2	1:E:182:CYS:HB2	2.52	0.44
1:D:362:HIS:CG	1:D:363:VAL:N	2.86	0.44
1:E:370:PHE:CD1	1:E:370:PHE:N	2.86	0.44
1:E:379:LEU:HB3	1:E:384:MET:HE1	1.99	0.44
1:B:112:VAL:HG21	1:C:254:ALA:HB2	2.00	0.43
1:B:391:ASN:CG	1:B:394:VAL:HG23	2.42	0.43
1:D:297:VAL:O	1:E:251:GLN:HA	2.18	0.43
1:E:153:LEU:HD12	1:E:153:LEU:C	2.43	0.43
1:E:161:PRO:HG2	1:E:192:ILE:HB	1.98	0.43
1:E:437:TYR:HB3	1:E:440:MET:HG3	1.99	0.43
1:A:114:VAL:HG21	1:B:290:HIS:HB3	2.00	0.43
1:A:359:TYR:CE2	1:B:265:GLY:HA3	2.53	0.43
1:B:259:ASN:ND2	1:B:259:ASN:C	2.74	0.43
1:B:391:ASN:OD1	1:B:394:VAL:HG23	2.18	0.43
1:D:259:ASN:ND2	1:D:259:ASN:C	2.76	0.43
1:E:174:ASN:O	1:E:175:THR:C	2.61	0.43
1:E:304:PHE:CE1	1:E:332:ASP:HB2	2.53	0.43
1:A:154:CYS:O	1:A:246:TYR:HA	2.18	0.43
1:A:397:ASP:O	1:A:399:ASN:N	2.51	0.43
1:B:358:GLU:HB2	1:C:287:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLU:HG2	1:C:188:ILE:HD12	1.99	0.43
1:C:197:MET:HE2	1:C:220:ASP:O	2.18	0.43
1:D:177:VAL:O	1:D:177:VAL:CG2	2.63	0.43
1:C:155:MET:HE1	1:C:229:PRO:HB3	1.99	0.43
1:C:391:ASN:OD1	1:C:394:VAL:HG23	2.17	0.43
1:D:246:TYR:CD1	1:D:246:TYR:C	2.96	0.43
1:A:177:VAL:O	1:A:177:VAL:CG2	2.65	0.43
1:A:245:PHE:CZ	1:A:308:TYR:HB3	2.53	0.43
1:B:122:LYS:HE3	1:B:258:PHE:CE2	2.54	0.43
1:B:359:TYR:CD2	1:C:182:CYS:HB2	2.53	0.43
1:C:157:GLY:O	1:C:326:LEU:HD23	2.19	0.43
1:C:174:ASN:HD22	1:C:174:ASN:HA	1.55	0.43
1:C:362:HIS:CG	1:C:363:VAL:N	2.87	0.43
1:C:397:ASP:O	1:C:399:ASN:N	2.51	0.43
1:D:245:PHE:CZ	1:D:308:TYR:HB3	2.53	0.43
1:D:304:PHE:CE1	1:D:332:ASP:HB2	2.54	0.43
1:B:66:GLN:NE2	1:B:68:ARG:NH2	2.66	0.43
1:B:156:VAL:HG12	1:B:157:GLY:N	2.33	0.43
1:B:434:GLN:NE2	1:B:435:ASP:H	2.17	0.43
1:D:243:LEU:O	1:D:243:LEU:HG	2.18	0.43
1:A:156:VAL:HG12	1:A:157:GLY:N	2.33	0.43
1:A:212:THR:HG21	1:E:344:SER:CB	2.48	0.43
1:B:344:SER:OG	1:C:212:THR:HG21	2.19	0.43
1:C:358:GLU:HB2	1:D:287:ILE:HD12	2.01	0.43
1:D:462:ARG:NH1	1:E:315:GLY:HA2	2.34	0.43
1:E:245:PHE:CZ	1:E:308:TYR:HB3	2.54	0.43
1:A:50:SER:C	1:A:51:ILE:HD12	2.43	0.43
1:A:114:VAL:CG2	1:B:290:HIS:HB3	2.48	0.43
1:B:111:GLY:HA2	1:C:252:MET:CE	2.49	0.43
1:B:360:MET:HE2	1:B:360:MET:HA	2.01	0.43
1:B:370:PHE:CD1	1:B:370:PHE:N	2.86	0.43
1:C:111:GLY:HA2	1:D:252:MET:HE1	1.99	0.43
1:D:391:ASN:OD1	1:D:394:VAL:HG23	2.19	0.43
1:E:380:SER:OG	1:E:383:VAL:HG23	2.19	0.43
1:E:391:ASN:OD1	1:E:394:VAL:HG23	2.18	0.43
1:B:23:THR:HG21	1:B:317:ASN:HA	2.01	0.43
1:C:370:PHE:CD1	1:C:370:PHE:N	2.86	0.43
1:A:297:VAL:O	1:B:251:GLN:HA	2.19	0.43
1:B:122:LYS:HG3	1:B:258:PHE:CD1	2.53	0.43
1:B:297:VAL:O	1:C:251:GLN:HA	2.18	0.43
1:C:68:ARG:HD3	1:C:68:ARG:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:CG2	1:D:290:HIS:HB3	2.49	0.43
1:E:122:LYS:HG3	1:E:258:PHE:CD1	2.54	0.43
1:B:23:THR:HA	1:B:26:TYR:CE2	2.54	0.42
1:C:289:VAL:CG1	1:C:290:HIS:N	2.81	0.42
1:D:296:LEU:HD12	1:E:251:GLN:HB2	2.01	0.42
1:A:263:THR:OG1	1:E:357:LYS:HG2	2.19	0.42
1:C:391:ASN:CG	1:C:394:VAL:HG23	2.43	0.42
1:C:462:ARG:HH11	1:D:315:GLY:HA2	1.82	0.42
1:D:51:ILE:O	1:D:51:ILE:HG22	2.19	0.42
1:B:362:HIS:CG	1:B:363:VAL:N	2.87	0.42
1:C:160:PRO:HB2	1:C:191:VAL:HG13	2.02	0.42
1:D:153:LEU:HD12	1:D:153:LEU:C	2.44	0.42
1:D:154:CYS:O	1:D:246:TYR:HA	2.19	0.42
1:A:51:ILE:HG12	1:B:266:GLU:CD	2.45	0.42
1:C:467:GLN:C	1:C:469:GLY:H	2.28	0.42
1:A:46:HIS:HB3	1:A:49:TYR:O	2.19	0.42
1:A:464:PHE:O	1:A:465:LEU:C	2.62	0.42
1:B:437:TYR:CD2	1:B:440:MET:SD	3.13	0.42
1:E:50:SER:C	1:E:51:ILE:HD12	2.45	0.42
1:E:467:GLN:C	1:E:469:GLY:H	2.27	0.42
1:A:122:LYS:HE3	1:A:258:PHE:CE2	2.54	0.42
1:C:51:ILE:HD12	1:C:51:ILE:N	2.35	0.42
1:E:246:TYR:CD1	1:E:246:TYR:C	2.98	0.42
1:B:352:THR:HB	1:B:355:ASP:OD1	2.20	0.42
1:C:296:LEU:HD12	1:D:251:GLN:HB2	2.01	0.42
1:D:123:TYR:CZ	1:D:136:PRO:HD3	2.55	0.42
1:D:150:GLN:NE2	1:D:297:VAL:HG12	2.35	0.42
1:D:256:HIS:O	1:D:290:HIS:HA	2.20	0.42
1:B:51:ILE:O	1:B:51:ILE:HG22	2.18	0.42
1:C:206:ASN:CG	1:C:225:VAL:HG22	2.44	0.42
1:C:256:HIS:O	1:C:290:HIS:HA	2.20	0.42
1:D:77:PRO:C	1:D:79:LYS:H	2.27	0.42
1:E:272:LEU:HA	1:E:272:LEU:HD23	1.84	0.42
1:A:127:GLU:OE1	1:E:255:ARG:NH1	2.53	0.42
1:B:177:VAL:O	1:B:178:GLN:C	2.62	0.42
1:B:206:ASN:CG	1:B:225:VAL:HG22	2.43	0.42
1:C:310:LEU:HD23	1:C:310:LEU:N	2.30	0.42
1:A:288:TYR:OH	1:E:143:ASN:ND2	2.52	0.41
1:A:305:ASN:HD22	1:A:305:ASN:HA	1.70	0.41
1:A:340:THR:OG1	1:A:360:MET:HE3	2.20	0.41
1:C:229:PRO:HB2	1:C:231:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:PRO:HB2	1:E:283:VAL:HG13	2.02	0.41
1:A:206:ASN:CG	1:A:225:VAL:HG22	2.45	0.41
1:B:178:GLN:O	1:B:179:ASN:C	2.63	0.41
1:D:206:ASN:CG	1:D:225:VAL:HG22	2.45	0.41
1:E:46:HIS:HB3	1:E:49:TYR:O	2.20	0.41
1:A:140:ASN:O	1:A:142:VAL:HG13	2.20	0.41
1:B:68:ARG:HA	1:B:68:ARG:HD3	1.80	0.41
1:B:77:PRO:C	1:B:79:LYS:H	2.27	0.41
1:B:143:ASN:ND2	1:C:288:TYR:OH	2.52	0.41
1:D:112:VAL:HG21	1:E:254:ALA:HB2	2.02	0.41
1:A:357:LYS:HG2	1:B:263:THR:OG1	2.21	0.41
1:B:358:GLU:HB2	1:C:287:ILE:CD1	2.50	0.41
1:B:234:MET:CB	1:B:243:LEU:HD22	2.49	0.41
1:C:376:SER:C	1:C:377:ILE:HG13	2.46	0.41
1:D:157:GLY:O	1:D:326:LEU:HD23	2.19	0.41
1:D:228:TYR:CD1	1:D:229:PRO:HD2	2.55	0.41
1:D:462:ARG:HH11	1:E:315:GLY:HA2	1.84	0.41
1:E:198:VAL:CG1	1:E:199:ASP:N	2.83	0.41
1:A:434:GLN:NE2	1:A:435:ASP:H	2.19	0.41
1:B:88:PHE:CD1	1:B:93:GLN:HG3	2.56	0.41
1:B:361:ARG:HD3	1:B:361:ARG:HA	1.91	0.41
1:D:317:ASN:OD1	1:D:317:ASN:C	2.62	0.41
1:D:467:GLN:C	1:D:469:GLY:H	2.28	0.41
1:E:140:ASN:O	1:E:142:VAL:HG13	2.21	0.41
1:B:467:GLN:C	1:B:469:GLY:H	2.28	0.41
1:C:198:VAL:CG1	1:C:199:ASP:N	2.83	0.41
1:C:259:ASN:ND2	1:C:260:ARG:N	2.65	0.41
1:C:277:GLY:O	1:C:278:ASN:CB	2.68	0.41
1:D:106:ARG:H	1:D:305:ASN:ND2	2.18	0.41
1:E:23:THR:HG23	1:E:316:HIS:O	2.21	0.41
1:E:464:PHE:O	1:E:465:LEU:C	2.62	0.41
1:A:161:PRO:HG2	1:A:192:ILE:HB	2.01	0.41
1:B:65:TYR:CZ	1:B:148:TYR:HB2	2.56	0.41
1:B:243:LEU:O	1:B:243:LEU:HG	2.21	0.41
1:B:246:TYR:CD1	1:B:246:TYR:C	2.98	0.41
1:C:156:VAL:HG12	1:C:157:GLY:N	2.36	0.41
1:C:462:ARG:NH1	1:D:315:GLY:HA2	2.36	0.41
1:E:206:ASN:CG	1:E:225:VAL:HG22	2.46	0.41
1:B:54:VAL:O	1:B:54:VAL:HG12	2.21	0.41
1:B:114:VAL:HG21	1:C:290:HIS:HB3	2.01	0.41
1:B:289:VAL:CG1	1:B:290:HIS:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:HG21	1:D:290:HIS:HB3	2.03	0.41
1:C:342:CYS:HB3	1:C:358:GLU:OE1	2.21	0.41
1:D:23:THR:HG23	1:D:317:ASN:HA	2.02	0.41
1:D:93:GLN:NE2	1:D:378:THR:HG22	2.36	0.41
1:E:154:CYS:O	1:E:246:TYR:HA	2.21	0.41
1:E:397:ASP:O	1:E:399:ASN:N	2.53	0.41
1:B:188:ILE:HD12	1:B:188:ILE:N	2.35	0.41
1:C:112:VAL:HG21	1:D:254:ALA:HB2	2.02	0.41
1:C:294:GLY:O	1:C:295:SER:O	2.39	0.41
1:D:397:ASP:O	1:D:399:ASN:N	2.54	0.41
1:A:89:ASP:C	1:A:91:THR:N	2.79	0.40
1:B:161:PRO:HG3	1:B:329:THR:OG1	2.21	0.40
1:C:70:PHE:CG	1:C:368:LEU:HD11	2.56	0.40
1:C:122:LYS:O	1:C:122:LYS:HD3	2.21	0.40
1:C:360:MET:HA	1:C:360:MET:HE2	2.03	0.40
1:D:177:VAL:O	1:D:178:GLN:C	2.64	0.40
1:D:256:HIS:CD2	1:E:128:ASN:ND2	2.89	0.40
1:A:288:TYR:CE1	1:E:116:GLY:HA3	2.56	0.40
1:D:89:ASP:C	1:D:91:THR:N	2.79	0.40
1:D:174:ASN:O	1:D:175:THR:C	2.64	0.40
1:D:259:ASN:HD22	1:D:259:ASN:C	2.26	0.40
1:A:106:ARG:H	1:A:305:ASN:ND2	2.15	0.40
1:A:123:TYR:CZ	1:A:136:PRO:HD3	2.57	0.40
1:A:177:VAL:O	1:A:178:GLN:C	2.62	0.40
1:A:259:ASN:ND2	1:A:260:ARG:N	2.68	0.40
1:D:94:ARG:HH11	1:D:94:ARG:HG2	1.85	0.40
1:D:140:ASN:O	1:D:142:VAL:HG13	2.21	0.40
1:D:358:GLU:HB2	1:E:287:ILE:HD12	2.03	0.40
1:E:256:HIS:O	1:E:290:HIS:HA	2.22	0.40
1:E:340:THR:OG1	1:E:360:MET:HE3	2.21	0.40
1:E:437:TYR:CD2	1:E:440:MET:SD	3.14	0.40
1:A:188:ILE:HD12	1:A:188:ILE:N	2.37	0.40
1:A:290:HIS:HB3	1:E:114:VAL:CG2	2.51	0.40
1:A:310:LEU:HD23	1:A:310:LEU:N	2.34	0.40
1:A:376:SER:C	1:A:377:ILE:HG13	2.46	0.40
1:C:76:ASP:OD1	1:C:76:ASP:C	2.64	0.40
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.91	0.40
1:E:70:PHE:CG	1:E:368:LEU:HD11	2.56	0.40
1:E:294:GLY:O	1:E:295:SER:O	2.39	0.40
1:B:33:PHE:CD2	1:B:373:GLN:HB2	2.57	0.40
1:B:87:LEU:O	1:B:88:PHE:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:CYS:HB3	1:B:358:GLU:OE1	2.21	0.40
1:B:357:LYS:HG2	1:C:263:THR:OG1	2.21	0.40
1:C:89:ASP:C	1:C:91:THR:N	2.79	0.40
1:C:116:GLY:HA3	1:D:288:TYR:CE1	2.57	0.40
1:C:174:ASN:O	1:C:175:THR:C	2.63	0.40
1:D:156:VAL:CG1	1:D:326:LEU:HD21	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	415/424 (98%)	351 (85%)	49 (12%)	15 (4%)	2	19
1	B	415/424 (98%)	350 (84%)	51 (12%)	14 (3%)	3	20
1	C	415/424 (98%)	352 (85%)	50 (12%)	13 (3%)	3	22
1	D	415/424 (98%)	352 (85%)	48 (12%)	15 (4%)	2	19
1	E	415/424 (98%)	351 (85%)	48 (12%)	16 (4%)	2	18
All	All	2075/2120 (98%)	1756 (85%)	246 (12%)	73 (4%)	3	20

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	LYS
1	B	295	SER
1	B	347	LYS
1	B	351	TYR
1	C	295	SER
1	C	347	LYS
1	C	351	TYR
1	D	295	SER

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Mol	Chain	Res	Type
1	D	347	LYS
1	D	351	TYR
1	E	295	SER
1	E	347	LYS
1	E	351	TYR
1	A	80	PHE
1	A	130	GLY
1	A	295	SER
1	A	351	TYR
1	B	130	GLY
1	B	348	SER
1	C	80	PHE
1	C	130	GLY
1	C	348	SER
1	D	80	PHE
1	D	130	GLY
1	D	348	SER
1	E	80	PHE
1	E	130	GLY
1	A	123	TYR
1	A	133	GLY
1	A	348	SER
1	B	80	PHE
1	B	123	TYR
1	B	398	TRP
1	C	123	TYR
1	E	123	TYR
1	E	348	SER
1	A	398	TRP
1	C	139	ASP
1	D	123	TYR
1	D	139	ASP
1	D	398	TRP
1	D	469	GLY
1	E	139	ASP
1	E	177	VAL
1	E	469	GLY
1	A	139	ASP
1	A	177	VAL
1	A	349	ALA
1	A	469	GLY
1	B	139	ASP

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Mol	Chain	Res	Type
1	B	469	GLY
1	C	177	VAL
1	C	218	PRO
1	C	469	GLY
1	D	87	LEU
1	D	177	VAL
1	E	87	LEU
1	E	218	PRO
1	E	398	TRP
1	A	218	PRO
1	B	218	PRO
1	D	218	PRO
1	E	349	ALA
1	B	133	GLY
1	B	177	VAL
1	E	54	VAL
1	A	54	VAL
1	C	54	VAL
1	B	54	VAL
1	D	54	VAL
1	C	108	GLN
1	D	108	GLN
1	E	108	GLN

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	364/365 (100%)	333 (92%)	31 (8%)	10	37
1	B	364/365 (100%)	332 (91%)	32 (9%)	9	35
1	C	364/365 (100%)	333 (92%)	31 (8%)	10	37
1	D	364/365 (100%)	334 (92%)	30 (8%)	10	39
1	E	364/365 (100%)	334 (92%)	30 (8%)	10	39
All	All	1820/1825 (100%)	1666 (92%)	154 (8%)	10	37

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	66	GLN
1	A	88	PHE
1	A	93	GLN
1	A	124	ASP
1	A	132	TYR
1	A	153	LEU
1	A	174	ASN
1	A	199	ASP
1	A	206	ASN
1	A	233	GLN
1	A	237	ASP
1	A	244	PHE
1	A	248	ARG
1	A	279	ASN
1	A	286	SER
1	A	310	LEU
1	A	314	GLN
1	A	326	LEU
1	A	337	THR
1	A	340	THR
1	A	341	LEU
1	A	350	THR
1	A	360	MET
1	A	364	GLU
1	A	433	LYS
1	A	440	MET
1	A	449	GLU
1	A	454	GLU
1	A	460	LEU
1	A	470	TYR
1	B	53	LYS
1	B	58	VAL
1	B	66	GLN
1	B	88	PHE
1	B	124	ASP
1	B	132	TYR
1	B	153	LEU
1	B	174	ASN
1	B	199	ASP
1	B	206	ASN
1	B	233	GLN

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Mol	Chain	Res	Type
1	B	237	ASP
1	B	244	PHE
1	B	248	ARG
1	B	273	LEU
1	B	279	ASN
1	B	286	SER
1	B	310	LEU
1	B	314	GLN
1	B	326	LEU
1	B	337	THR
1	B	340	THR
1	B	341	LEU
1	B	350	THR
1	B	360	MET
1	B	364	GLU
1	B	433	LYS
1	B	440	MET
1	B	449	GLU
1	B	454	GLU
1	B	460	LEU
1	B	470	TYR
1	C	53	LYS
1	C	66	GLN
1	C	88	PHE
1	C	124	ASP
1	C	132	TYR
1	C	153	LEU
1	C	174	ASN
1	C	199	ASP
1	C	206	ASN
1	C	233	GLN
1	C	237	ASP
1	C	244	PHE
1	C	248	ARG
1	C	273	LEU
1	C	279	ASN
1	C	286	SER
1	C	310	LEU
1	C	314	GLN
1	C	326	LEU
1	C	337	THR
1	C	340	THR

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Mol	Chain	Res	Type
1	C	341	LEU
1	C	350	THR
1	C	360	MET
1	C	361	ARG
1	C	433	LYS
1	C	440	MET
1	C	449	GLU
1	C	454	GLU
1	C	460	LEU
1	C	470	TYR
1	D	53	LYS
1	D	66	GLN
1	D	88	PHE
1	D	124	ASP
1	D	132	TYR
1	D	153	LEU
1	D	174	ASN
1	D	199	ASP
1	D	206	ASN
1	D	233	GLN
1	D	237	ASP
1	D	244	PHE
1	D	248	ARG
1	D	273	LEU
1	D	279	ASN
1	D	286	SER
1	D	310	LEU
1	D	314	GLN
1	D	326	LEU
1	D	337	THR
1	D	340	THR
1	D	341	LEU
1	D	350	THR
1	D	360	MET
1	D	433	LYS
1	D	440	MET
1	D	449	GLU
1	D	454	GLU
1	D	460	LEU
1	D	470	TYR
1	E	53	LYS
1	E	66	GLN

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Mol	Chain	Res	Type
1	E	88	PHE
1	E	124	ASP
1	E	132	TYR
1	E	153	LEU
1	E	174	ASN
1	E	199	ASP
1	E	206	ASN
1	E	233	GLN
1	E	237	ASP
1	E	248	ARG
1	E	273	LEU
1	E	279	ASN
1	E	286	SER
1	E	310	LEU
1	E	314	GLN
1	E	326	LEU
1	E	337	THR
1	E	340	THR
1	E	341	LEU
1	E	350	THR
1	E	360	MET
1	E	364	GLU
1	E	433	LYS
1	E	440	MET
1	E	449	GLU
1	E	454	GLU
1	E	460	LEU
1	E	470	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	66	GLN
1	A	135	ASN
1	A	140	ASN
1	A	143	ASN
1	A	150	GLN
1	A	165	HIS
1	A	174	ASN
1	A	179	ASN
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	256	HIS
1	A	259	ASN
1	A	290	HIS
1	A	305	ASN
1	A	318	ASN
1	A	324	ASN
1	A	338	ASN
1	A	353	ASN
1	A	362	HIS
1	A	369	GLN
1	A	391	ASN
1	A	399	ASN
1	A	434	GLN
1	A	457	GLN
1	B	31	ASN
1	B	66	GLN
1	B	135	ASN
1	B	140	ASN
1	B	143	ASN
1	B	150	GLN
1	B	165	HIS
1	B	174	ASN
1	B	179	ASN
1	B	206	ASN
1	B	233	GLN
1	B	256	HIS
1	B	259	ASN
1	B	290	HIS
1	B	305	ASN
1	B	316	HIS
1	B	318	ASN
1	B	324	ASN
1	B	338	ASN
1	B	353	ASN
1	B	362	HIS
1	B	369	GLN
1	B	391	ASN
1	B	399	ASN
1	B	434	GLN
1	B	457	GLN
1	C	31	ASN

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Mol	Chain	Res	Type
1	C	66	GLN
1	C	135	ASN
1	C	140	ASN
1	C	143	ASN
1	C	150	GLN
1	C	165	HIS
1	C	174	ASN
1	C	179	ASN
1	C	206	ASN
1	C	233	GLN
1	C	256	HIS
1	C	259	ASN
1	C	290	HIS
1	C	305	ASN
1	C	318	ASN
1	C	324	ASN
1	C	338	ASN
1	C	353	ASN
1	C	362	HIS
1	C	369	GLN
1	C	391	ASN
1	C	399	ASN
1	C	434	GLN
1	C	457	GLN
1	D	31	ASN
1	D	66	GLN
1	D	135	ASN
1	D	140	ASN
1	D	143	ASN
1	D	150	GLN
1	D	165	HIS
1	D	174	ASN
1	D	179	ASN
1	D	206	ASN
1	D	233	GLN
1	D	256	HIS
1	D	259	ASN
1	D	305	ASN
1	D	318	ASN
1	D	324	ASN
1	D	353	ASN
1	D	362	HIS

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Mol	Chain	Res	Type
1	D	369	GLN
1	D	391	ASN
1	D	399	ASN
1	D	434	GLN
1	D	457	GLN
1	E	31	ASN
1	E	66	GLN
1	E	135	ASN
1	E	140	ASN
1	E	143	ASN
1	E	150	GLN
1	E	165	HIS
1	E	174	ASN
1	E	179	ASN
1	E	206	ASN
1	E	233	GLN
1	E	256	HIS
1	E	259	ASN
1	E	290	HIS
1	E	305	ASN
1	E	316	HIS
1	E	318	ASN
1	E	324	ASN
1	E	338	ASN
1	E	353	ASN
1	E	362	HIS
1	E	369	GLN
1	E	391	ASN
1	E	399	ASN
1	E	434	GLN
1	E	457	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	419/424 (98%)	1.17	74 (17%) 4 3	3, 4, 6, 9	0
1	B	419/424 (98%)	1.00	67 (15%) 5 3	3, 4, 6, 7	0
1	C	419/424 (98%)	1.10	72 (17%) 4 3	3, 4, 6, 7	0
1	D	419/424 (98%)	1.08	77 (18%) 3 3	3, 4, 6, 7	0
1	E	419/424 (98%)	1.13	75 (17%) 3 3	3, 4, 6, 7	0
All	All	2095/2120 (98%)	1.10	365 (17%) 4 3	3, 4, 6, 9	0

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ASN	8.9
1	E	130	GLY	8.0
1	A	130	GLY	7.9
1	A	85	SER	7.8
1	E	434	GLN	7.1
1	C	167	GLY	6.8
1	E	172	SER	6.7
1	A	175	THR	6.6
1	D	84	ASP	6.4
1	B	83	PRO	6.3
1	C	83	PRO	6.3
1	C	434	GLN	6.3
1	E	348	SER	6.3
1	A	84	ASP	6.2
1	A	53	LYS	6.1
1	B	84	ASP	6.1
1	E	87	LEU	5.8
1	A	355	ASP	5.8
1	A	83	PRO	5.8
1	C	348	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	452	SER	5.7
1	D	111	GLY	5.6
1	C	435	ASP	5.5
1	D	172	SER	5.5
1	D	83	PRO	5.2
1	E	54	VAL	5.2
1	A	177	VAL	5.1
1	B	80	PHE	5.1
1	B	173	SER	5.0
1	B	175	THR	5.0
1	A	54	VAL	5.0
1	C	87	LEU	5.0
1	B	31	ASN	5.0
1	E	55	ASN	4.9
1	D	130	GLY	4.9
1	A	470	TYR	4.9
1	A	81	ALA	4.9
1	C	172	SER	4.8
1	A	399	ASN	4.8
1	D	82	LEU	4.8
1	C	54	VAL	4.8
1	B	85	SER	4.7
1	E	86	SER	4.7
1	A	82	LEU	4.7
1	E	347	LYS	4.7
1	D	347	LYS	4.7
1	C	349	ALA	4.7
1	E	84	ASP	4.7
1	C	44	VAL	4.6
1	A	435	ASP	4.6
1	E	83	PRO	4.5
1	D	81	ALA	4.5
1	C	85	SER	4.4
1	B	87	LEU	4.3
1	E	470	TYR	4.3
1	C	31	ASN	4.2
1	C	55	ASN	4.2
1	E	176	SER	4.2
1	A	80	PHE	4.2
1	E	454	GLU	4.2
1	B	86	SER	4.1
1	C	380	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	91	THR	4.1
1	B	245	PHE	4.0
1	B	349	ALA	4.0
1	A	276	GLY	4.0
1	B	434	GLN	4.0
1	E	107	GLY	4.0
1	D	174	ASN	4.0
1	C	198	VAL	3.9
1	C	147	ASP	3.9
1	D	144	VAL	3.9
1	A	172	SER	3.9
1	A	135	ASN	3.8
1	A	279	ASN	3.8
1	A	131	GLY	3.8
1	D	470	TYR	3.8
1	D	131	GLY	3.8
1	E	19	ALA	3.7
1	C	129	SER	3.7
1	D	176	SER	3.7
1	D	437	TYR	3.7
1	E	57	THR	3.7
1	B	176	SER	3.7
1	B	55	ASN	3.7
1	A	134	GLY	3.7
1	C	113	GLY	3.7
1	E	469	GLY	3.7
1	C	347	LYS	3.6
1	E	131	GLY	3.6
1	C	436	PRO	3.6
1	B	350	THR	3.6
1	D	177	VAL	3.6
1	E	81	ALA	3.6
1	D	289	VAL	3.5
1	E	279	ASN	3.5
1	C	56	LYS	3.5
1	E	223	GLY	3.5
1	D	76	ASP	3.5
1	B	82	LEU	3.4
1	B	137	GLY	3.4
1	D	80	PHE	3.4
1	B	314	GLN	3.4
1	D	175	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	439	ASP	3.4
1	D	87	LEU	3.4
1	D	163	GLY	3.4
1	D	399	ASN	3.4
1	D	245	PHE	3.4
1	E	173	SER	3.4
1	E	82	LEU	3.4
1	A	145	GLY	3.4
1	D	138	GLN	3.4
1	B	54	VAL	3.3
1	B	342	CYS	3.3
1	E	363	VAL	3.3
1	E	437	TYR	3.3
1	E	175	THR	3.3
1	E	350	THR	3.3
1	E	338	ASN	3.3
1	B	437	TYR	3.3
1	A	345	VAL	3.3
1	C	382	GLU	3.3
1	A	147	ASP	3.3
1	C	439	ASP	3.3
1	D	383	VAL	3.3
1	A	157	GLY	3.3
1	C	294	GLY	3.3
1	D	258	PHE	3.2
1	D	115	SER	3.2
1	E	315	GLY	3.2
1	C	388	HIS	3.2
1	E	286	SER	3.2
1	E	116	GLY	3.1
1	A	308	TYR	3.1
1	B	238	PRO	3.1
1	A	391	ASN	3.1
1	E	134	GLY	3.1
1	A	438	LYS	3.1
1	C	175	THR	3.1
1	E	177	VAL	3.1
1	E	258	PHE	3.1
1	D	53	LYS	3.1
1	E	56	LYS	3.1
1	B	348	SER	3.0
1	D	55	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	325	HIS	3.0
1	A	176	SER	3.0
1	B	308	TYR	3.0
1	C	270	ASP	3.0
1	B	36	ALA	3.0
1	A	350	THR	3.0
1	D	22	ALA	3.0
1	A	124	ASP	3.0
1	A	397	ASP	3.0
1	E	435	ASP	3.0
1	E	111	GLY	3.0
1	D	434	GLN	3.0
1	C	174	ASN	3.0
1	B	81	ALA	2.9
1	D	444	GLU	2.9
1	D	159	ALA	2.9
1	C	363	VAL	2.9
1	A	101	GLY	2.9
1	D	441	SER	2.9
1	C	325	HIS	2.9
1	E	278	ASN	2.9
1	A	258	PHE	2.9
1	C	88	PHE	2.9
1	A	362	HIS	2.9
1	B	88	PHE	2.9
1	B	438	LYS	2.8
1	D	188	ILE	2.8
1	E	236	ALA	2.8
1	E	77	PRO	2.8
1	E	324	ASN	2.8
1	C	460	LEU	2.8
1	A	434	GLN	2.8
1	A	105	GLY	2.8
1	C	384	MET	2.8
1	D	314	GLN	2.8
1	A	25	ALA	2.8
1	C	354	SER	2.8
1	C	58	VAL	2.7
1	E	91	THR	2.7
1	B	399	ASN	2.7
1	D	54	VAL	2.7
1	E	283	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	171	GLN	2.7
1	A	203	GLY	2.7
1	B	107	GLY	2.7
1	B	167	GLY	2.7
1	E	25	ALA	2.7
1	C	338	ASN	2.7
1	E	340	THR	2.7
1	C	133	GLY	2.6
1	D	186	GLU	2.6
1	A	352	THR	2.6
1	A	39	SER	2.6
1	C	82	LEU	2.6
1	E	349	ALA	2.6
1	B	325	HIS	2.6
1	B	302	GLN	2.6
1	E	171	GLN	2.6
1	B	277	GLY	2.6
1	A	454	GLU	2.6
1	A	375	CYS	2.6
1	D	284	ALA	2.6
1	E	73	VAL	2.6
1	E	329	THR	2.6
1	A	360	MET	2.6
1	A	271	ASP	2.6
1	A	55	ASN	2.6
1	E	44	VAL	2.6
1	D	348	SER	2.6
1	A	277	GLY	2.6
1	B	135	ASN	2.6
1	E	72	VAL	2.6
1	B	464	PHE	2.5
1	B	171	GLN	2.5
1	C	449	GLU	2.5
1	B	119	LEU	2.5
1	B	294	GLY	2.5
1	A	33	PHE	2.5
1	B	323	GLY	2.5
1	C	114	VAL	2.5
1	A	278	ASN	2.5
1	D	209	ASP	2.5
1	D	317	ASN	2.5
1	A	183	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	168	LYS	2.5
1	A	237	ASP	2.5
1	A	305	ASN	2.5
1	A	353	ASN	2.5
1	A	200	THR	2.5
1	B	170	THR	2.5
1	C	131	GLY	2.5
1	E	196	ASP	2.4
1	C	148	TYR	2.4
1	B	469	GLY	2.4
1	A	275	LYS	2.4
1	C	433	LYS	2.4
1	D	143	ASN	2.4
1	C	84	ASP	2.4
1	D	261	ALA	2.4
1	D	382	GLU	2.4
1	B	37	SER	2.4
1	B	174	ASN	2.4
1	C	334	THR	2.4
1	E	170	THR	2.4
1	E	333	THR	2.4
1	B	468	SER	2.4
1	B	337	THR	2.4
1	A	133	GLY	2.4
1	A	240	GLY	2.4
1	A	437	TYR	2.4
1	B	382	GLU	2.4
1	C	217	VAL	2.4
1	E	151	THR	2.3
1	C	53	LYS	2.3
1	C	357	LYS	2.3
1	D	381	ALA	2.3
1	E	65	TYR	2.3
1	E	76	ASP	2.3
1	D	366	PHE	2.3
1	D	396	GLU	2.3
1	A	354	SER	2.3
1	E	85	SER	2.3
1	B	276	GLY	2.3
1	A	325	HIS	2.3
1	B	132	TYR	2.3
1	E	31	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	174	ASN	2.3
1	D	39	SER	2.3
1	A	87	LEU	2.3
1	C	135	ASN	2.3
1	C	138	GLN	2.3
1	C	364	GLU	2.3
1	D	294	GLY	2.3
1	C	381	ALA	2.3
1	D	19	ALA	2.3
1	A	348	SER	2.3
1	E	326	LEU	2.3
1	C	179	ASN	2.3
1	C	317	ASN	2.3
1	E	121	ASN	2.3
1	B	347	LYS	2.3
1	A	59	VAL	2.3
1	A	349	ALA	2.3
1	C	469	GLY	2.3
1	D	95	LEU	2.3
1	D	129	SER	2.3
1	A	433	LYS	2.3
1	B	44	VAL	2.3
1	A	340	THR	2.2
1	D	85	SER	2.2
1	B	124	ASP	2.2
1	E	444	GLU	2.2
1	D	469	GLY	2.2
1	C	437	TYR	2.2
1	A	173	SER	2.2
1	A	359	TYR	2.2
1	C	318	ASN	2.2
1	B	130	GLY	2.2
1	D	133	GLY	2.2
1	E	433	LYS	2.2
1	A	244	PHE	2.2
1	E	88	PHE	2.2
1	D	114	VAL	2.2
1	D	308	TYR	2.2
1	E	237	ASP	2.2
1	D	467	GLN	2.1
1	E	153	LEU	2.1
1	C	22	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	295	SER	2.1
1	D	86	SER	2.1
1	D	349	ALA	2.1
1	D	354	SER	2.1
1	B	179	ASN	2.1
1	D	305	ASN	2.1
1	E	436	PRO	2.1
1	B	147	ASP	2.1
1	D	367	ASP	2.1
1	B	114	VAL	2.1
1	B	189	THR	2.1
1	B	344	SER	2.1
1	C	258	PHE	2.1
1	B	237	ASP	2.1
1	C	383	VAL	2.1
1	D	363	VAL	2.1
1	E	439	ASP	2.1
1	C	263	THR	2.1
1	C	233	GLN	2.1
1	D	235	ALA	2.1
1	B	64	GLY	2.1
1	D	134	GLY	2.1
1	C	391	ASN	2.1
1	A	24	ASP	2.1
1	B	89	ASP	2.1
1	D	435	ASP	2.1
1	C	186	GLU	2.1
1	B	453	SER	2.1
1	E	346	SER	2.1
1	C	291	THR	2.1
1	C	385	ALA	2.1
1	D	171	GLN	2.1
1	E	314	GLN	2.1
1	B	345	VAL	2.0
1	E	445	VAL	2.0
1	D	173	SER	2.0
1	B	318	ASN	2.0
1	E	135	ASN	2.0
1	D	316	HIS	2.0
1	B	439	ASP	2.0
1	C	38	SER	2.0
1	C	173	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	287	ILE	2.0
1	D	140	ASN	2.0
1	D	259	ASN	2.0
1	A	107	GLY	2.0
1	A	56	LYS	2.0
1	D	233	GLN	2.0
1	E	238	PRO	2.0
1	B	444	GLU	2.0
1	C	268	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.