



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:32 PM UTC

PDB ID : 1ELO / pdb_00001elo
Title : ELONGATION FACTOR G WITHOUT NUCLEOTIDE
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Deposited on : 1996-03-13
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

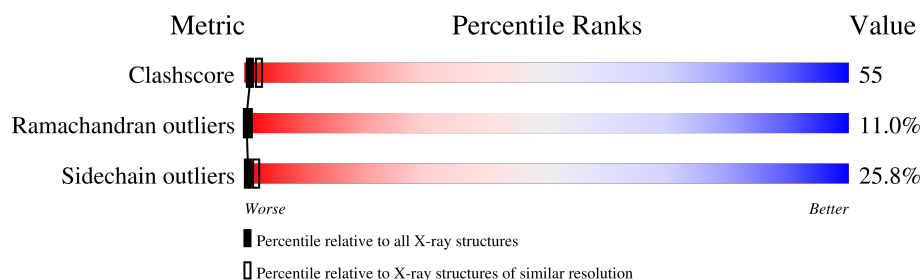
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	691	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4957 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 ELONGATION FACTOR G.

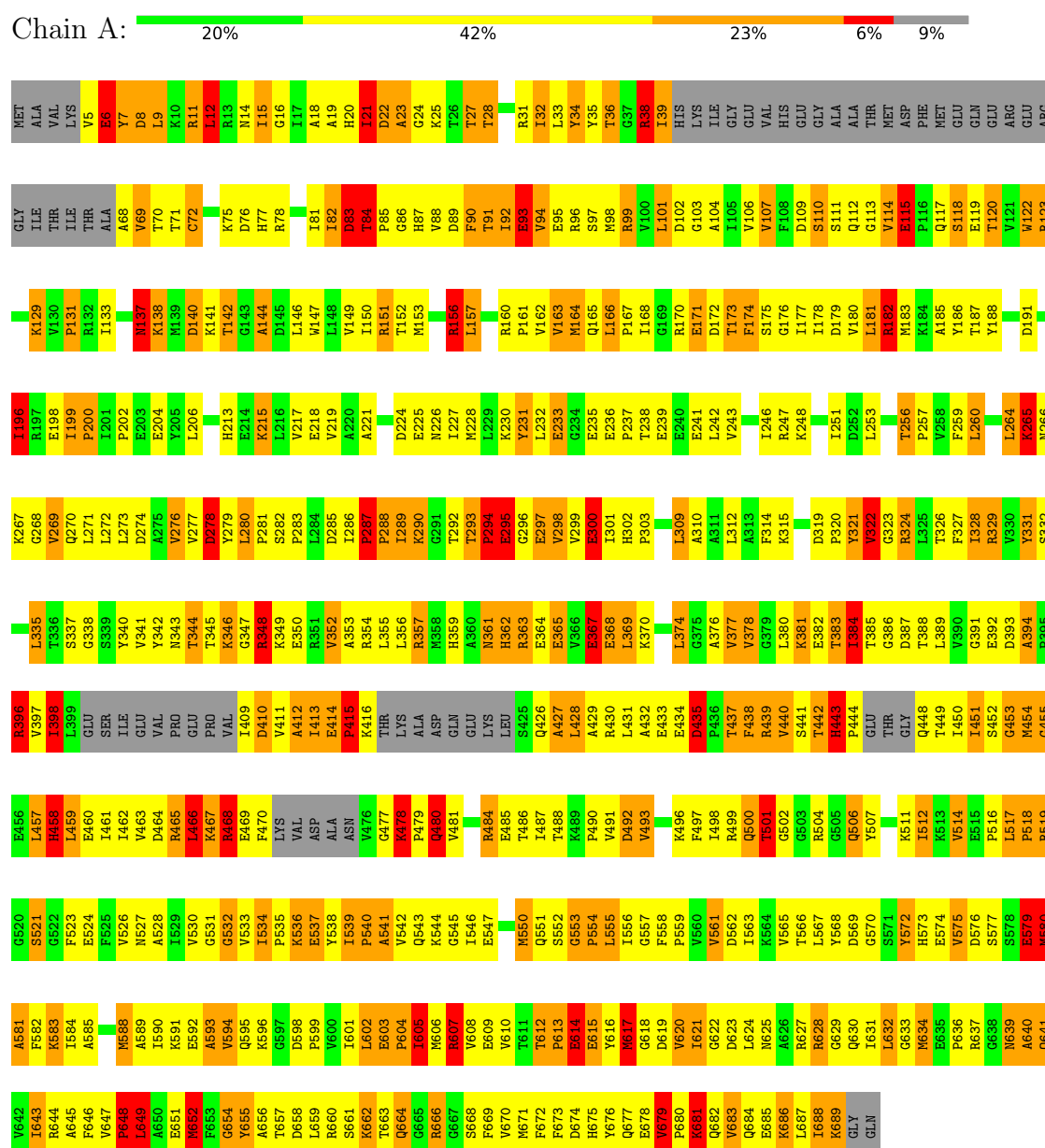
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	632	4957	3157	849	933	18	0	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: ELONGATION FACTOR G



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.60Å 106.00Å 116.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4957	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	11/5048 (0.2%)	1.59	110/6829 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	580	MET	SD-CE	8.80	2.01	1.79
1	A	164	MET	SD-CE	-8.72	1.57	1.79
1	A	440	VAL	CA-CB	6.94	1.61	1.53
1	A	256	THR	CA-CB	6.67	1.60	1.53
1	A	289	ILE	CA-CB	6.41	1.61	1.54
1	A	163	VAL	CA-CB	5.78	1.59	1.53
1	A	588	MET	SD-CE	5.62	1.93	1.79
1	A	634	MET	SD-CE	5.61	1.93	1.79
1	A	617	MET	SD-CE	5.42	1.93	1.79
1	A	173	THR	CA-CB	5.32	1.62	1.53
1	A	501	THR	CA-CB	5.25	1.62	1.53

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	THR	CA-C-N	-14.57	104.77	119.78
1	A	293	THR	C-N-CA	-14.57	104.77	119.78
1	A	458	HIS	N-CA-C	-13.29	96.33	112.54
1	A	466	LEU	N-CA-C	-12.87	96.39	108.75
1	A	278	ASP	N-CA-C	11.48	123.79	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	VAL	N-CA-C	-10.73	101.47	111.67
1	A	465	ARG	N-CA-C	-10.10	99.77	113.30
1	A	588	MET	N-CA-C	-10.01	99.91	112.72
1	A	15	ILE	N-CA-C	9.65	122.66	108.96
1	A	459	LEU	N-CA-C	-9.42	100.71	110.97
1	A	615	GLU	N-CA-C	9.39	123.77	111.75
1	A	22	ASP	N-CA-C	9.06	120.85	110.97
1	A	613	PRO	N-CA-C	-9.04	97.00	111.19
1	A	398	ILE	N-CA-C	-8.86	95.06	107.99
1	A	295	GLU	N-CA-C	-8.77	92.13	110.80
1	A	534	ILE	N-CA-C	-8.53	90.45	108.88
1	A	579	GLU	N-CA-C	-8.53	101.34	112.68
1	A	349	LYS	N-CA-C	-8.22	96.57	109.72
1	A	412	ALA	N-CA-C	8.12	128.11	110.80
1	A	493	VAL	N-CA-C	7.94	125.85	109.34
1	A	294	PRO	N-CA-C	7.79	123.61	111.21
1	A	521	SER	N-CA-C	-7.77	100.25	110.43
1	A	300	GLU	N-CA-C	7.73	122.14	107.75
1	A	156	ARG	N-CA-C	7.69	119.74	111.36
1	A	552	SER	N-CA-C	7.65	123.67	107.67
1	A	115	GLU	N-CA-C	-7.62	99.57	110.08
1	A	287	PRO	CA-C-N	7.60	129.34	119.84
1	A	287	PRO	C-N-CA	7.60	129.34	119.84
1	A	200	PRO	N-CA-C	-7.56	98.40	111.32
1	A	553	GLY	CA-C-N	7.52	129.24	119.84
1	A	553	GLY	C-N-CA	7.52	129.24	119.84
1	A	8	ASP	N-CA-C	-7.50	96.40	108.55
1	A	367	GLU	N-CA-C	7.43	122.37	113.16
1	A	443	HIS	N-CA-C	7.37	126.09	109.81
1	A	583	LYS	N-CA-C	-7.34	103.94	113.12
1	A	441	SER	N-CA-C	7.08	120.49	109.52
1	A	28	THR	N-CA-C	-7.05	104.15	112.89
1	A	21	ILE	CB-CA-C	-6.90	99.97	111.29
1	A	361	ASN	N-CA-C	6.89	118.26	108.54
1	A	265	LYS	N-CA-C	-6.85	104.46	114.39
1	A	628	ARG	N-CA-C	-6.80	104.56	112.86
1	A	231	TYR	N-CA-C	-6.79	103.80	111.14
1	A	386	GLY	N-CA-C	-6.73	105.82	115.64
1	A	478	LYS	N-CA-C	6.30	123.73	109.81
1	A	294	PRO	CB-CA-C	6.27	119.25	111.23
1	A	282	SER	N-CA-C	-6.26	102.79	110.31
1	A	480	GLN	N-CA-C	6.21	119.31	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	VAL	N-CA-C	-6.17	99.59	108.48
1	A	21	ILE	CA-C-N	6.16	128.78	120.65
1	A	21	ILE	C-N-CA	6.16	128.78	120.65
1	A	451	ILE	N-CA-C	-6.14	100.79	109.63
1	A	620	VAL	N-CA-C	-6.12	105.18	110.74
1	A	500	GLN	N-CA-C	-6.11	105.62	114.12
1	A	290	LYS	N-CA-C	-6.10	102.66	110.53
1	A	541	ALA	N-CA-C	-6.02	104.78	111.71
1	A	605	ILE	N-CA-C	-5.99	101.81	109.30
1	A	553	GLY	N-CA-C	5.97	124.51	112.34
1	A	394	ALA	CA-C-N	5.95	127.28	119.84
1	A	394	ALA	C-N-CA	5.95	127.28	119.84
1	A	679	VAL	N-CA-C	-5.92	96.09	108.88
1	A	122	TRP	N-CA-C	-5.92	104.74	111.07
1	A	512	ILE	N-CA-C	5.84	115.95	108.82
1	A	219	VAL	CB-CA-C	-5.83	104.17	112.22
1	A	103	GLY	N-CA-C	-5.83	104.16	112.55
1	A	592	GLU	N-CA-C	-5.81	104.64	110.97
1	A	581	ALA	N-CA-C	-5.81	106.33	113.41
1	A	346	LYS	N-CA-C	5.78	122.33	113.19
1	A	561	VAL	N-CA-C	5.75	115.83	108.82
1	A	414	GLU	N-CA-C	5.72	120.19	107.95
1	A	607	ARG	N-CA-C	-5.71	97.56	107.49
1	A	202	PRO	N-CA-C	-5.69	102.27	111.03
1	A	666	ARG	N-CA-C	-5.68	106.24	112.72
1	A	603	GLU	N-CA-C	5.67	113.32	108.22
1	A	686	LYS	N-CA-C	-5.67	103.93	111.24
1	A	344	THR	CB-CA-C	-5.64	101.96	110.92
1	A	603	GLU	CA-C-N	5.62	126.87	119.84
1	A	603	GLU	C-N-CA	5.62	126.87	119.84
1	A	492	ASP	N-CA-CB	-5.62	101.75	110.57
1	A	539	ILE	CA-C-N	5.59	124.94	118.85
1	A	539	ILE	C-N-CA	5.59	124.94	118.85
1	A	36	THR	N-CA-C	-5.57	104.43	111.11
1	A	453	GLY	N-CA-C	5.56	126.36	113.18
1	A	545	GLY	N-CA-C	-5.47	106.16	112.73
1	A	654	GLY	N-CA-C	-5.46	108.58	115.08
1	A	215	LYS	N-CA-C	-5.45	105.42	111.36
1	A	182	ARG	N-CA-C	-5.42	107.03	113.97
1	A	12	LEU	N-CA-C	5.42	118.09	107.57
1	A	228	MET	N-CA-C	-5.40	105.29	111.07
1	A	396	ARG	N-CA-C	5.38	117.48	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ALA	N-CA-C	5.37	122.24	110.80
1	A	593	ALA	CA-C-N	-5.37	116.24	122.63
1	A	593	ALA	C-N-CA	-5.37	116.24	122.63
1	A	363	ARG	N-CA-C	-5.33	103.49	110.53
1	A	84	THR	CA-C-N	5.30	125.36	119.32
1	A	84	THR	C-N-CA	5.30	125.36	119.32
1	A	604	PRO	N-CA-C	5.30	123.38	112.47
1	A	478	LYS	CA-C-N	-5.28	113.24	119.84
1	A	478	LYS	C-N-CA	-5.28	113.24	119.84
1	A	91	THR	N-CA-C	5.22	121.91	110.80
1	A	152	THR	N-CA-C	5.20	116.95	111.28
1	A	428	LEU	N-CA-C	5.17	121.82	110.80
1	A	199	ILE	CA-C-N	5.12	125.51	119.99
1	A	199	ILE	C-N-CA	5.12	125.51	119.99
1	A	394	ALA	N-CA-C	-5.08	102.66	110.07
1	A	35	TYR	N-CA-C	5.06	116.88	111.36
1	A	9	LEU	N-CA-C	-5.05	106.38	112.54
1	A	328	ILE	CB-CA-C	-5.05	104.84	111.70
1	A	280	LEU	N-CA-C	5.04	116.18	109.93
1	A	77	HIS	CA-C-N	-5.01	116.11	122.77
1	A	77	HIS	C-N-CA	-5.01	116.11	122.77

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	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	4957	0	5021	546	0
All	All	4957	0	5021	546	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:MET:SD	1:A:580:MET:CE	2.01	1.48
1:A:346:LYS:HD3	1:A:384:ILE:HD11	1.46	0.97
1:A:289:ILE:HG23	1:A:301:ILE:HB	1.45	0.97
1:A:457:LEU:HG	1:A:460:GLU:HB2	1.45	0.96
1:A:6:GLU:HG2	1:A:7:TYR:H	1.32	0.94
1:A:528:ALA:HB3	1:A:568:TYR:HA	1.51	0.93
1:A:9:LEU:HD21	1:A:303:PRO:HB2	1.49	0.92
1:A:335:LEU:HD21	1:A:355:LEU:HD21	1.51	0.91
1:A:213:HIS:O	1:A:217:VAL:HG23	1.73	0.87
1:A:92:ILE:HD11	1:A:454:MET:SD	2.14	0.87
1:A:87:HIS:NE2	1:A:90:PHE:HB2	1.90	0.86
1:A:85:PRO:HG3	1:A:94:VAL:HA	1.58	0.86
1:A:156:ARG:HD2	1:A:666:ARG:HH12	1.39	0.85
1:A:535:PRO:HD3	1:A:572:TYR:CD2	2.13	0.84
1:A:99:ARG:HD3	1:A:99:ARG:O	1.77	0.84
1:A:493:VAL:HG21	1:A:593:ALA:HB2	1.60	0.84
1:A:444:PRO:HA	1:A:448:GLN:HG3	1.59	0.83
1:A:628:ARG:HD2	1:A:648:PRO:HG2	1.61	0.82
1:A:671:MET:C	1:A:672:PHE:HD1	1.87	0.82
1:A:511:LYS:HD2	1:A:569:ASP:HB3	1.61	0.81
1:A:290:LYS:HB3	1:A:298:VAL:HG12	1.62	0.81
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.44	0.80
1:A:411:VAL:HB	1:A:453:GLY:HA3	1.61	0.80
1:A:27:THR:O	1:A:31:ARG:HG2	1.82	0.80
1:A:411:VAL:HB	1:A:453:GLY:CA	2.12	0.79
1:A:439:ARG:HB2	1:A:439:ARG:HH11	1.47	0.79
1:A:499:ARG:HG3	1:A:499:ARG:HH11	1.46	0.78
1:A:359:HIS:HB2	1:A:362:HIS:O	1.83	0.77
1:A:346:LYS:NZ	1:A:383:THR:HA	1.99	0.77
1:A:247:ARG:HG3	1:A:279:TYR:HA	1.65	0.77
1:A:156:ARG:HD2	1:A:666:ARG:NH1	2.00	0.76
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.51	0.76
1:A:478:LYS:O	1:A:480:GLN:HG3	1.87	0.75
1:A:120:THR:HA	1:A:123:ARG:HG3	1.69	0.75
1:A:624:LEU:HD23	1:A:631:ILE:HD11	1.67	0.75
1:A:610:VAL:HG13	1:A:659:LEU:HD21	1.68	0.74
1:A:647:VAL:HG11	1:A:652:MET:SD	2.27	0.74
1:A:296:GLY:O	1:A:297:GLU:HB2	1.86	0.74
1:A:434:GLU:O	1:A:435:ASP:HB2	1.87	0.74
1:A:481:VAL:HG13	1:A:649:LEU:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:GLN:HB2	1:A:646:PHE:HB2	1.68	0.74
1:A:346:LYS:HZ2	1:A:383:THR:HA	1.53	0.74
1:A:176:GLY:HA2	1:A:187:THR:HA	1.70	0.73
1:A:276:VAL:HG13	1:A:280:LEU:HD12	1.69	0.73
1:A:658:ASP:O	1:A:662:LYS:HG2	1.88	0.73
1:A:160:ARG:HG3	1:A:160:ARG:HH11	1.53	0.73
1:A:309:LEU:HG	1:A:310:ALA:N	2.03	0.73
1:A:129:LYS:O	1:A:131:PRO:HD3	1.89	0.73
1:A:539:ILE:HB	1:A:540:PRO:HD3	1.69	0.73
1:A:484:ARG:HB2	1:A:602:LEU:HB2	1.71	0.73
1:A:468:ARG:HA	1:A:468:ARG:NE	2.05	0.72
1:A:606:MET:HE2	1:A:649:LEU:HD23	1.69	0.72
1:A:170:ARG:H	1:A:173:THR:HB	1.54	0.72
1:A:6:GLU:HG2	1:A:7:TYR:N	2.04	0.72
1:A:535:PRO:HD3	1:A:572:TYR:HD2	1.52	0.72
1:A:577:SER:HB3	1:A:582:PHE:HE1	1.54	0.72
1:A:413:ILE:HD11	1:A:454:MET:O	1.89	0.71
1:A:181:LEU:HD12	1:A:181:LEU:O	1.90	0.71
1:A:514:VAL:HG21	1:A:593:ALA:HB1	1.71	0.71
1:A:621:ILE:HD11	1:A:643:ILE:HG21	1.71	0.71
1:A:673:PHE:CZ	1:A:675:HIS:HA	2.26	0.71
1:A:85:PRO:CG	1:A:94:VAL:HA	2.20	0.71
1:A:426:GLN:HE21	1:A:430:ARG:NH2	1.88	0.71
1:A:519:ARG:HH11	1:A:519:ARG:HB2	1.54	0.71
1:A:68:ALA:O	1:A:69:VAL:HG23	1.91	0.71
1:A:613:PRO:HA	1:A:640:ALA:CB	2.21	0.71
1:A:348:ARG:NH2	1:A:381:LYS:HE3	2.05	0.71
1:A:344:THR:OG1	1:A:388:THR:HB	1.91	0.70
1:A:290:LYS:HA	1:A:299:VAL:O	1.91	0.70
1:A:346:LYS:HE3	1:A:382:GLU:O	1.92	0.70
1:A:185:ALA:HB3	1:A:199:ILE:HG13	1.74	0.70
1:A:608:VAL:HG21	1:A:652:MET:HE1	1.74	0.70
1:A:591:LYS:O	1:A:595:GLN:HG2	1.92	0.70
1:A:439:ARG:HH11	1:A:439:ARG:CB	2.05	0.69
1:A:680:PRO:O	1:A:683:VAL:HG23	1.92	0.69
1:A:274:ASP:O	1:A:278:ASP:HB2	1.91	0.69
1:A:5:VAL:HG22	1:A:6:GLU:N	2.08	0.69
1:A:617:MET:O	1:A:617:MET:SD	2.50	0.69
1:A:636:PRO:HA	1:A:641:GLN:HG2	1.75	0.69
1:A:92:ILE:O	1:A:93:GLU:HB2	1.91	0.69
1:A:612:THR:O	1:A:640:ALA:HB1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG22	1:A:6:GLU:H	1.58	0.68
1:A:613:PRO:HA	1:A:640:ALA:HB2	1.73	0.68
1:A:321:TYR:O	1:A:322:VAL:HG22	1.93	0.68
1:A:191:ASP:HA	1:A:265:LYS:O	1.93	0.68
1:A:580:MET:O	1:A:584:ILE:HD13	1.93	0.68
1:A:9:LEU:HD21	1:A:303:PRO:CB	2.23	0.68
1:A:239:GLU:O	1:A:243:VAL:HG23	1.93	0.68
1:A:409:ILE:O	1:A:411:VAL:N	2.27	0.68
1:A:493:VAL:HG23	1:A:512:ILE:HG13	1.76	0.68
1:A:185:ALA:HB3	1:A:199:ILE:CG1	2.24	0.67
1:A:416:LYS:HG2	1:A:449:THR:HB	1.76	0.67
1:A:90:PHE:CE2	1:A:458:HIS:HA	2.30	0.67
1:A:438:PHE:O	1:A:439:ARG:HG3	1.93	0.67
1:A:164:MET:HE1	1:A:246:ILE:HG21	1.75	0.66
1:A:504:ARG:HG2	1:A:504:ARG:HH11	1.60	0.66
1:A:396:ARG:H	1:A:396:ARG:HE	1.43	0.66
1:A:607:ARG:NH1	1:A:672:PHE:HB2	2.10	0.66
1:A:679:VAL:HG13	1:A:683:VAL:HB	1.77	0.66
1:A:614:GLU:OE1	1:A:641:GLN:HG3	1.96	0.66
1:A:466:LEU:O	1:A:468:ARG:N	2.29	0.65
1:A:92:ILE:HD13	1:A:92:ILE:H	1.59	0.65
1:A:413:ILE:HD12	1:A:459:LEU:HD11	1.78	0.65
1:A:14:ASN:HD22	1:A:329:ARG:HH21	1.44	0.65
1:A:34:TYR:CD1	1:A:34:TYR:C	2.75	0.64
1:A:357:ARG:HH11	1:A:357:ARG:CG	2.11	0.64
1:A:462:ILE:O	1:A:466:LEU:HB2	1.96	0.64
1:A:70:THR:HG22	1:A:71:THR:H	1.62	0.64
1:A:528:ALA:HB3	1:A:568:TYR:CA	2.26	0.64
1:A:443:HIS:O	1:A:448:GLN:N	2.30	0.64
1:A:14:ASN:HD22	1:A:329:ARG:NH2	1.96	0.64
1:A:147:TRP:O	1:A:151:ARG:HB2	1.98	0.64
1:A:309:LEU:HG	1:A:310:ALA:H	1.60	0.64
1:A:627:ARG:O	1:A:647:VAL:HG23	1.98	0.64
1:A:348:ARG:CZ	1:A:382:GLU:HG3	2.28	0.63
1:A:621:ILE:O	1:A:621:ILE:HG22	1.98	0.63
1:A:459:LEU:HD12	1:A:459:LEU:H	1.64	0.63
1:A:90:PHE:HE2	1:A:458:HIS:CA	2.12	0.63
1:A:27:THR:HG22	1:A:31:ARG:HG2	1.81	0.62
1:A:34:TYR:O	1:A:34:TYR:HD1	1.82	0.62
1:A:115:GLU:HG2	1:A:118:SER:OG	1.99	0.62
1:A:517:LEU:HD23	1:A:518:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:HA	1:A:470:PHE:CE2	2.34	0.62
1:A:97:SER:O	1:A:101:LEU:HD22	1.99	0.62
1:A:168:ILE:HD11	1:A:178:ILE:HD11	1.81	0.62
1:A:439:ARG:CB	1:A:439:ARG:NH1	2.63	0.61
1:A:458:HIS:HA	1:A:461:ILE:HG13	1.82	0.61
1:A:526:VAL:HG12	1:A:527:ASN:N	2.15	0.61
1:A:555:LEU:HD11	1:A:599:PRO:HB2	1.81	0.61
1:A:467:LYS:HG2	1:A:467:LYS:O	2.00	0.61
1:A:348:ARG:HH22	1:A:381:LYS:HE3	1.64	0.61
1:A:468:ARG:HA	1:A:468:ARG:CZ	2.31	0.60
1:A:499:ARG:HG3	1:A:499:ARG:NH1	2.15	0.60
1:A:232:LEU:O	1:A:233:GLU:HB2	2.01	0.60
1:A:295:GLU:O	1:A:295:GLU:HG3	2.02	0.60
1:A:71:THR:O	1:A:72:CYS:HB2	2.01	0.60
1:A:355:LEU:HD23	1:A:377:VAL:HA	1.83	0.60
1:A:19:ALA:HB2	1:A:107:VAL:CG1	2.31	0.60
1:A:9:LEU:CD2	1:A:303:PRO:HB2	2.27	0.59
1:A:87:HIS:CE1	1:A:90:PHE:HB2	2.36	0.59
1:A:129:LYS:HG2	1:A:253:LEU:HD11	1.82	0.59
1:A:616:TYR:CD2	1:A:663:THR:HB	2.36	0.59
1:A:457:LEU:CG	1:A:460:GLU:HB2	2.26	0.59
1:A:517:LEU:HD22	1:A:521:SER:HB3	1.85	0.59
1:A:34:TYR:CD1	1:A:34:TYR:O	2.55	0.59
1:A:454:MET:HG2	1:A:455:GLY:H	1.68	0.59
1:A:413:ILE:CD1	1:A:459:LEU:HD11	2.31	0.59
1:A:497:PHE:O	1:A:498:ILE:HD12	2.02	0.59
1:A:546:ILE:HD13	1:A:565:VAL:HG11	1.84	0.59
1:A:628:ARG:HH11	1:A:648:PRO:HB2	1.67	0.59
1:A:91:THR:HA	1:A:94:VAL:HB	1.84	0.59
1:A:265:LYS:HB3	1:A:267:LYS:HZ3	1.67	0.59
1:A:356:LEU:HD23	1:A:365:GLU:HA	1.83	0.59
1:A:681:LYS:N	1:A:681:LYS:CD	2.66	0.59
1:A:294:PRO:HD3	1:A:398:ILE:HD11	1.84	0.59
1:A:309:LEU:HA	1:A:332:SER:O	2.03	0.58
1:A:468:ARG:HH11	1:A:468:ARG:HG2	1.67	0.58
1:A:647:VAL:CG1	1:A:652:MET:SD	2.91	0.58
1:A:188:TYR:CE2	1:A:268:GLY:N	2.70	0.58
1:A:639:ASN:OD1	1:A:640:ALA:N	2.36	0.58
1:A:481:VAL:HG22	1:A:649:LEU:HD13	1.86	0.58
1:A:177:ILE:HD12	1:A:188:TYR:HE2	1.67	0.58
1:A:497:PHE:CG	1:A:584:ILE:HG21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:HB3	1:A:434:GLU:OE1	2.02	0.58
1:A:498:ILE:HD11	1:A:507:TYR:CE2	2.39	0.58
1:A:684:GLN:O	1:A:688:ILE:HG12	2.03	0.58
1:A:204:GLU:OE1	1:A:204:GLU:N	2.37	0.58
1:A:78:ARG:CZ	1:A:357:ARG:HH21	2.17	0.58
1:A:75:LYS:O	1:A:76:ASP:HB3	2.03	0.57
1:A:342:TYR:CD1	1:A:348:ARG:O	2.57	0.57
1:A:160:ARG:HH11	1:A:160:ARG:CG	2.18	0.57
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.69	0.57
1:A:343:ASN:OD1	1:A:346:LYS:HB2	2.03	0.57
1:A:342:TYR:CE1	1:A:347:GLY:O	2.58	0.57
1:A:442:THR:O	1:A:448:GLN:N	2.38	0.57
1:A:681:LYS:H	1:A:681:LYS:HD2	1.70	0.57
1:A:165:GLN:HG3	1:A:260:LEU:HD13	1.87	0.57
1:A:196:ILE:HG12	1:A:196:ILE:O	2.04	0.56
1:A:454:MET:HB3	1:A:458:HIS:CD2	2.40	0.56
1:A:624:LEU:HD23	1:A:631:ILE:CD1	2.34	0.56
1:A:164:MET:CE	1:A:246:ILE:HG21	2.35	0.56
1:A:218:GLU:HG3	1:A:231:TYR:CE2	2.40	0.56
1:A:661:SER:OG	1:A:662:LYS:HD3	2.05	0.56
1:A:109:ASP:OD1	1:A:138:LYS:HD2	2.05	0.56
1:A:427:ALA:HA	1:A:470:PHE:CD2	2.41	0.56
1:A:427:ALA:CB	1:A:470:PHE:HD2	2.18	0.56
1:A:181:LEU:HD21	1:A:243:VAL:HG22	1.88	0.56
1:A:498:ILE:HD11	1:A:507:TYR:CD2	2.41	0.55
1:A:556:ILE:HD13	1:A:601:ILE:HD13	1.88	0.55
1:A:22:ASP:C	1:A:24:GLY:N	2.60	0.55
1:A:430:ARG:C	1:A:432:ALA:H	2.14	0.55
1:A:32:ILE:HG22	1:A:33:LEU:N	2.21	0.55
1:A:416:LYS:HA	1:A:449:THR:O	2.07	0.55
1:A:469:GLU:O	1:A:470:PHE:HD1	1.88	0.55
1:A:98:MET:HA	1:A:101:LEU:CD2	2.36	0.55
1:A:119:GLU:O	1:A:122:TRP:HB3	2.05	0.55
1:A:345:THR:HG23	1:A:388:THR:H	1.70	0.55
1:A:605:ILE:HD13	1:A:677:GLN:HB3	1.89	0.55
1:A:439:ARG:NH1	1:A:439:ARG:HB3	2.21	0.55
1:A:512:ILE:HG12	1:A:589:ALA:HB1	1.89	0.55
1:A:486:THR:HG22	1:A:487:ILE:O	2.06	0.55
1:A:491:VAL:HG11	1:A:596:LYS:O	2.07	0.55
1:A:188:TYR:CD2	1:A:267:LYS:HA	2.41	0.55
1:A:335:LEU:HD11	1:A:352:VAL:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:VAL:C	1:A:622:GLY:H	2.15	0.55
1:A:523:PHE:CD1	1:A:524:GLU:N	2.75	0.55
1:A:22:ASP:O	1:A:24:GLY:N	2.40	0.54
1:A:342:TYR:HE1	1:A:347:GLY:O	1.90	0.54
1:A:342:TYR:HD1	1:A:348:ARG:O	1.90	0.54
1:A:341:VAL:HG23	1:A:350:GLU:HB2	1.87	0.54
1:A:646:PHE:O	1:A:648:PRO:HD3	2.07	0.54
1:A:328:ILE:HD11	1:A:369:LEU:HD11	1.89	0.54
1:A:415:PRO:HD2	1:A:451:ILE:O	2.07	0.54
1:A:539:ILE:CB	1:A:540:PRO:HD3	2.38	0.54
1:A:511:LYS:CD	1:A:569:ASP:HB3	2.36	0.54
1:A:90:PHE:CE2	1:A:458:HIS:CA	2.90	0.54
1:A:484:ARG:O	1:A:485:GLU:HG2	2.07	0.54
1:A:572:TYR:HB3	1:A:582:PHE:HZ	1.73	0.54
1:A:69:VAL:CG2	1:A:314:PHE:HZ	2.20	0.54
1:A:272:LEU:O	1:A:276:VAL:HG23	2.08	0.54
1:A:107:VAL:HG23	1:A:137:ASN:HB2	1.89	0.54
1:A:431:LEU:O	1:A:438:PHE:HE2	1.89	0.54
1:A:610:VAL:HG22	1:A:669:PHE:HB3	1.90	0.54
1:A:286:ILE:HG22	1:A:287:PRO:N	2.22	0.54
1:A:488:THR:OG1	1:A:598:ASP:HB2	2.07	0.54
1:A:616:TYR:OH	1:A:664:GLN:NE2	2.41	0.54
1:A:81:ILE:O	1:A:81:ILE:HG22	2.08	0.53
1:A:411:VAL:HB	1:A:453:GLY:HA2	1.91	0.53
1:A:460:GLU:O	1:A:463:VAL:HB	2.08	0.53
1:A:31:ARG:HD2	1:A:31:ARG:N	2.23	0.53
1:A:265:LYS:HB3	1:A:267:LYS:NZ	2.23	0.53
1:A:500:GLN:C	1:A:502:GLY:N	2.67	0.53
1:A:70:THR:HG22	1:A:71:THR:N	2.24	0.53
1:A:368:GLU:O	1:A:368:GLU:HG3	2.09	0.53
1:A:292:THR:O	1:A:398:ILE:HD12	2.09	0.53
1:A:340:TYR:HB2	1:A:392:GLU:OE2	2.09	0.53
1:A:78:ARG:NH2	1:A:357:ARG:HH21	2.07	0.53
1:A:290:LYS:HB3	1:A:298:VAL:CG1	2.37	0.53
1:A:671:MET:C	1:A:672:PHE:CD1	2.78	0.53
1:A:343:ASN:ND2	1:A:383:THR:OG1	2.41	0.53
1:A:460:GLU:HA	1:A:463:VAL:CG2	2.39	0.52
1:A:609:GLU:O	1:A:669:PHE:HA	2.10	0.52
1:A:345:THR:OG1	1:A:387:ASP:OD1	2.27	0.52
1:A:377:VAL:HG22	1:A:377:VAL:O	2.08	0.52
1:A:465:ARG:HA	1:A:469:GLU:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:HZ3	1:A:583:LYS:HZ3	1.57	0.52
1:A:608:VAL:HG12	1:A:610:VAL:HG23	1.91	0.52
1:A:276:VAL:CG1	1:A:280:LEU:HD12	2.38	0.52
1:A:608:VAL:HG21	1:A:652:MET:CE	2.39	0.52
1:A:572:TYR:N	1:A:572:TYR:CD1	2.76	0.52
1:A:187:THR:O	1:A:187:THR:HG23	2.10	0.52
1:A:319:ASP:CG	1:A:363:ARG:HH22	2.18	0.52
1:A:457:LEU:HA	1:A:460:GLU:H	1.74	0.52
1:A:462:ILE:HG22	1:A:466:LEU:HD13	1.91	0.52
1:A:465:ARG:HA	1:A:469:GLU:HB3	1.90	0.52
1:A:517:LEU:HD22	1:A:521:SER:CB	2.40	0.52
1:A:624:LEU:CD2	1:A:631:ILE:HD11	2.38	0.52
1:A:610:VAL:HG22	1:A:669:PHE:CB	2.39	0.52
1:A:643:ILE:O	1:A:643:ILE:HG12	2.10	0.52
1:A:87:HIS:O	1:A:89:ASP:N	2.43	0.52
1:A:398:ILE:HD12	1:A:398:ILE:H	1.74	0.51
1:A:25:LYS:NZ	1:A:84:THR:OG1	2.43	0.51
1:A:227:ILE:HG23	1:A:237:PRO:HG2	1.93	0.51
1:A:497:PHE:CD1	1:A:584:ILE:HG21	2.46	0.51
1:A:315:LYS:O	1:A:327:PHE:HB2	2.10	0.51
1:A:514:VAL:CG2	1:A:593:ALA:HB1	2.38	0.51
1:A:526:VAL:CG1	1:A:527:ASN:N	2.74	0.51
1:A:329:ARG:HG2	1:A:331:TYR:CZ	2.45	0.51
1:A:608:VAL:CG1	1:A:610:VAL:HG23	2.41	0.51
1:A:613:PRO:O	1:A:615:GLU:N	2.43	0.51
1:A:624:LEU:HD23	1:A:631:ILE:CG1	2.41	0.51
1:A:246:ILE:HG22	1:A:246:ILE:O	2.11	0.51
1:A:319:ASP:CG	1:A:363:ARG:HH12	2.19	0.51
1:A:348:ARG:NE	1:A:382:GLU:HG3	2.25	0.51
1:A:457:LEU:C	1:A:459:LEU:N	2.63	0.51
1:A:98:MET:HA	1:A:101:LEU:HD22	1.91	0.51
1:A:528:ALA:N	1:A:567:LEU:O	2.43	0.51
1:A:577:SER:HB3	1:A:582:PHE:CE1	2.41	0.50
1:A:685:GLU:HA	1:A:688:ILE:HD11	1.93	0.50
1:A:411:VAL:HG21	1:A:439:ARG:HD3	1.93	0.50
1:A:555:LEU:CD1	1:A:599:PRO:HB2	2.41	0.50
1:A:630:GLN:O	1:A:631:ILE:C	2.51	0.50
1:A:170:ARG:N	1:A:173:THR:HB	2.23	0.50
1:A:514:VAL:HG21	1:A:593:ALA:CB	2.41	0.50
1:A:179:ASP:OD2	1:A:182:ARG:HB2	2.11	0.50
1:A:603:GLU:HB2	1:A:604:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:HG22	1:A:256:THR:O	2.12	0.50
1:A:329:ARG:CD	1:A:374:LEU:HD23	2.41	0.50
1:A:573:HIS:HB3	1:A:576:ASP:H	1.76	0.50
1:A:607:ARG:HA	1:A:645:ALA:O	2.12	0.50
1:A:140:ASP:HA	1:A:171:GLU:HA	1.94	0.50
1:A:357:ARG:CG	1:A:357:ARG:NH1	2.68	0.50
1:A:361:ASN:O	1:A:362:HIS:CB	2.59	0.50
1:A:110:SER:HB2	1:A:137:ASN:O	2.12	0.49
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.25	0.49
1:A:572:TYR:O	1:A:572:TYR:HD1	1.95	0.49
1:A:269:VAL:O	1:A:270:GLN:C	2.55	0.49
1:A:413:ILE:HA	1:A:480:GLN:O	2.12	0.49
1:A:430:ARG:C	1:A:432:ALA:N	2.68	0.49
1:A:435:ASP:C	1:A:437:THR:H	2.19	0.49
1:A:572:TYR:CD1	1:A:572:TYR:C	2.90	0.49
1:A:361:ASN:O	1:A:362:HIS:HB3	2.10	0.49
1:A:519:ARG:HB2	1:A:519:ARG:NH1	2.25	0.49
1:A:530:VAL:O	1:A:530:VAL:HG23	2.12	0.49
1:A:671:MET:O	1:A:672:PHE:HD1	1.94	0.49
1:A:377:VAL:HG22	1:A:380:LEU:HD12	1.93	0.49
1:A:500:GLN:O	1:A:502:GLY:N	2.46	0.49
1:A:554:PRO:HB3	1:A:595:GLN:HE21	1.76	0.49
1:A:443:HIS:HB2	1:A:450:ILE:HD13	1.95	0.49
1:A:500:GLN:C	1:A:502:GLY:H	2.21	0.49
1:A:434:GLU:OE1	1:A:434:GLU:N	2.45	0.49
1:A:517:LEU:CD2	1:A:518:PRO:HD2	2.43	0.49
1:A:604:PRO:HG2	1:A:649:LEU:HB3	1.95	0.49
1:A:411:VAL:O	1:A:453:GLY:HA2	2.12	0.49
1:A:558:PHE:HB3	1:A:559:PRO:HD2	1.94	0.49
1:A:269:VAL:HG23	1:A:270:GLN:OE1	2.13	0.49
1:A:301:ILE:HG23	1:A:332:SER:HB2	1.93	0.49
1:A:409:ILE:C	1:A:411:VAL:H	2.20	0.49
1:A:119:GLU:HG3	1:A:157:LEU:HD12	1.94	0.49
1:A:344:THR:HG22	1:A:396:ARG:HB2	1.95	0.49
1:A:450:ILE:O	1:A:450:ILE:HG13	2.13	0.49
1:A:182:ARG:O	1:A:183:MET:HB2	2.13	0.48
1:A:344:THR:HG21	1:A:397:VAL:N	2.27	0.48
1:A:465:ARG:C	1:A:469:GLU:HB3	2.38	0.48
1:A:348:ARG:NH2	1:A:382:GLU:HG3	2.28	0.48
1:A:523:PHE:CD1	1:A:550:MET:HE1	2.48	0.48
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:HZ3	1:A:583:LYS:NZ	2.11	0.48
1:A:477:GLY:C	1:A:479:PRO:HD3	2.38	0.48
1:A:607:ARG:HH11	1:A:672:PHE:HB2	1.76	0.48
1:A:19:ALA:HB2	1:A:107:VAL:HG12	1.96	0.48
1:A:438:PHE:CD1	1:A:439:ARG:N	2.82	0.48
1:A:547:GLU:O	1:A:547:GLU:HG2	2.14	0.48
1:A:553:GLY:O	1:A:557:GLY:HA2	2.12	0.48
1:A:156:ARG:NH1	1:A:666:ARG:HH11	2.11	0.48
1:A:329:ARG:HA	1:A:374:LEU:HB3	1.95	0.48
1:A:314:PHE:CD1	1:A:315:LYS:HB2	2.49	0.48
1:A:392:GLU:HG3	1:A:392:GLU:O	2.14	0.48
1:A:661:SER:OG	1:A:662:LYS:N	2.44	0.48
1:A:20:HIS:NE2	1:A:21:ILE:HG13	2.29	0.48
1:A:162:VAL:HG12	1:A:163:VAL:N	2.28	0.48
1:A:188:TYR:OH	1:A:271:LEU:HD12	2.14	0.48
1:A:415:PRO:O	1:A:450:ILE:HA	2.13	0.48
1:A:171:GLU:CG	1:A:172:ASP:H	2.27	0.47
1:A:329:ARG:HD3	1:A:331:TYR:OH	2.13	0.47
1:A:528:ALA:HB3	1:A:567:LEU:O	2.14	0.47
1:A:227:ILE:HG23	1:A:237:PRO:CG	2.44	0.47
1:A:542:VAL:O	1:A:544:LYS:N	2.47	0.47
1:A:554:PRO:HG2	1:A:594:VAL:HB	1.96	0.47
1:A:329:ARG:HH11	1:A:329:ARG:CG	2.26	0.47
1:A:22:ASP:C	1:A:24:GLY:H	2.21	0.47
1:A:286:ILE:CG2	1:A:287:PRO:N	2.78	0.47
1:A:20:HIS:ND1	1:A:117:GLN:OE1	2.47	0.47
1:A:141:LYS:O	1:A:142:THR:C	2.57	0.47
1:A:243:VAL:HG13	1:A:279:TYR:CE1	2.50	0.47
1:A:493:VAL:HG23	1:A:512:ILE:CG1	2.43	0.47
1:A:91:THR:O	1:A:94:VAL:N	2.48	0.47
1:A:114:VAL:HG12	1:A:114:VAL:O	2.13	0.47
1:A:168:ILE:HD11	1:A:178:ILE:CD1	2.44	0.47
1:A:22:ASP:O	1:A:23:ALA:C	2.55	0.47
1:A:153:MET:HA	1:A:157:LEU:HD22	1.96	0.47
1:A:319:ASP:HB3	1:A:322:VAL:HG22	1.97	0.47
1:A:344:THR:HG1	1:A:388:THR:HB	1.78	0.47
1:A:367:GLU:O	1:A:368:GLU:HB3	2.15	0.47
1:A:616:TYR:O	1:A:618:GLY:N	2.45	0.47
1:A:343:ASN:OD1	1:A:346:LYS:N	2.48	0.47
1:A:506:GLN:HA	1:A:576:ASP:O	2.15	0.47
1:A:672:PHE:CD1	1:A:672:PHE:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:O	1:A:92:ILE:HG12	2.12	0.47
1:A:410:ASP:O	1:A:411:VAL:HG22	2.15	0.47
1:A:637:ARG:HG2	1:A:637:ARG:HH11	1.80	0.47
1:A:120:THR:HG21	1:A:668:SER:HB3	1.96	0.47
1:A:140:ASP:HB3	1:A:174:PHE:HD2	1.79	0.47
1:A:465:ARG:CA	1:A:469:GLU:HB3	2.45	0.46
1:A:669:PHE:HE2	1:A:671:MET:HE2	1.80	0.46
1:A:328:ILE:HG12	1:A:377:VAL:HG12	1.97	0.46
1:A:469:GLU:C	1:A:470:PHE:HD1	2.23	0.46
1:A:613:PRO:HG3	1:A:666:ARG:HH21	1.79	0.46
1:A:8:ASP:HB3	1:A:11:ARG:HG2	1.97	0.46
1:A:90:PHE:CE2	1:A:461:ILE:HD11	2.50	0.46
1:A:309:LEU:CG	1:A:310:ALA:N	2.75	0.46
1:A:323:GLY:O	1:A:324:ARG:C	2.58	0.46
1:A:534:ILE:HD11	1:A:570:GLY:HA3	1.98	0.46
1:A:614:GLU:H	1:A:614:GLU:HG2	1.53	0.46
1:A:627:ARG:HA	1:A:651:GLU:HG2	1.98	0.46
1:A:300:GLU:HG2	1:A:302:HIS:HE1	1.81	0.46
1:A:354:ARG:HG3	1:A:378:VAL:HG12	1.98	0.46
1:A:499:ARG:HG3	1:A:501:THR:H	1.80	0.46
1:A:572:TYR:CD1	1:A:572:TYR:O	2.68	0.46
1:A:573:HIS:ND1	1:A:576:ASP:HB2	2.30	0.46
1:A:329:ARG:NH1	1:A:331:TYR:CE1	2.84	0.46
1:A:588:MET:O	1:A:589:ALA:C	2.59	0.46
1:A:176:GLY:CA	1:A:187:THR:HA	2.44	0.46
1:A:294:PRO:O	1:A:295:GLU:HB3	2.16	0.46
1:A:416:LYS:HG2	1:A:449:THR:CB	2.45	0.46
1:A:608:VAL:HG12	1:A:609:GLU:N	2.31	0.46
1:A:133:ILE:HD12	1:A:259:PHE:CE2	2.51	0.46
1:A:160:ARG:CG	1:A:160:ARG:NH1	2.77	0.46
1:A:185:ALA:HB3	1:A:199:ILE:HG12	1.97	0.46
1:A:620:VAL:O	1:A:624:LEU:HB2	2.17	0.45
1:A:146:LEU:HD12	1:A:167:PRO:HD2	1.98	0.45
1:A:357:ARG:HD3	1:A:364:GLU:OE2	2.16	0.45
1:A:512:ILE:CD1	1:A:589:ALA:HB1	2.46	0.45
1:A:357:ARG:O	1:A:359:HIS:HD2	1.99	0.45
1:A:628:ARG:CD	1:A:648:PRO:HG2	2.41	0.45
1:A:38:ARG:CG	1:A:39:ILE:H	2.29	0.45
1:A:342:TYR:HE1	1:A:347:GLY:C	2.25	0.45
1:A:416:LYS:HG2	1:A:449:THR:CG2	2.46	0.45
1:A:490:PRO:HG3	1:A:516:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:PHE:HD1	1:A:672:PHE:N	2.14	0.45
1:A:584:ILE:HG22	1:A:585:ALA:N	2.32	0.45
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.59	0.45
1:A:85:PRO:HG3	1:A:94:VAL:CA	2.39	0.45
1:A:90:PHE:O	1:A:94:VAL:HG23	2.17	0.45
1:A:102:ASP:HB3	1:A:286:ILE:HD11	1.97	0.45
1:A:270:GLN:O	1:A:273:LEU:N	2.47	0.45
1:A:518:PRO:HB2	1:A:521:SER:OG	2.16	0.45
1:A:542:VAL:O	1:A:543:GLN:C	2.60	0.45
1:A:605:ILE:HG13	1:A:648:PRO:HG3	1.98	0.45
1:A:688:ILE:O	1:A:689:LYS:HD3	2.16	0.45
1:A:20:HIS:O	1:A:21:ILE:C	2.59	0.45
1:A:238:THR:OG1	1:A:241:GLU:HB2	2.17	0.45
1:A:544:LYS:NZ	1:A:583:LYS:NZ	2.63	0.45
1:A:674:ASP:O	1:A:675:HIS:HB3	2.17	0.45
1:A:69:VAL:HG21	1:A:314:PHE:HZ	1.81	0.45
1:A:536:LYS:HA	1:A:539:ILE:HD12	1.99	0.45
1:A:613:PRO:HG3	1:A:666:ARG:HE	1.82	0.45
1:A:319:ASP:CG	1:A:320:PRO:HD2	2.42	0.45
1:A:364:GLU:O	1:A:364:GLU:HG2	2.17	0.45
1:A:627:ARG:HB3	1:A:647:VAL:HG21	1.98	0.45
1:A:553:GLY:HA2	1:A:554:PRO:HD3	1.81	0.44
1:A:659:LEU:HD12	1:A:659:LEU:HA	1.76	0.44
1:A:632:LEU:HG	1:A:633:GLY:N	2.32	0.44
1:A:146:LEU:HD12	1:A:167:PRO:CD	2.48	0.44
1:A:361:ASN:O	1:A:362:HIS:ND1	2.50	0.44
1:A:112:GLN:O	1:A:113:GLY:C	2.60	0.44
1:A:129:LYS:O	1:A:129:LYS:CD	2.65	0.44
1:A:427:ALA:O	1:A:429:ALA:N	2.51	0.44
1:A:539:ILE:O	1:A:543:GLN:HG3	2.18	0.44
1:A:687:LEU:HD23	1:A:687:LEU:HA	1.77	0.44
1:A:82:ILE:O	1:A:83:ASP:C	2.59	0.44
1:A:129:LYS:O	1:A:129:LYS:CG	2.65	0.44
1:A:538:TYR:O	1:A:541:ALA:N	2.51	0.44
1:A:16:GLY:HA3	1:A:101:LEU:HD12	1.99	0.44
1:A:186:TYR:CE1	1:A:198:GLU:HG2	2.53	0.43
1:A:604:PRO:O	1:A:649:LEU:HB2	2.18	0.43
1:A:114:VAL:O	1:A:156:ARG:NH2	2.51	0.43
1:A:119:GLU:OE2	1:A:123:ARG:NH1	2.52	0.43
1:A:162:VAL:CG1	1:A:163:VAL:N	2.82	0.43
1:A:176:GLY:HA2	1:A:186:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PRO:HB2	1:A:300:GLU:HG3	1.99	0.43
1:A:579:GLU:C	1:A:581:ALA:H	2.26	0.43
1:A:651:GLU:O	1:A:652:MET:HB2	2.18	0.43
1:A:199:ILE:HB	1:A:200:PRO:HD2	2.00	0.43
1:A:579:GLU:O	1:A:581:ALA:N	2.50	0.43
1:A:621:ILE:O	1:A:621:ILE:CG2	2.65	0.43
1:A:5:VAL:CG2	1:A:6:GLU:N	2.78	0.43
1:A:20:HIS:CD2	1:A:21:ILE:HG13	2.54	0.43
1:A:146:LEU:O	1:A:149:VAL:HB	2.18	0.43
1:A:427:ALA:HB2	1:A:470:PHE:HD2	1.82	0.43
1:A:535:PRO:O	1:A:537:GLU:N	2.52	0.43
1:A:11:ARG:HG2	1:A:11:ARG:H	1.63	0.43
1:A:156:ARG:HH11	1:A:666:ARG:HH11	1.66	0.43
1:A:224:ASP:O	1:A:225:GLU:C	2.61	0.43
1:A:354:ARG:HG3	1:A:378:VAL:CG1	2.49	0.43
1:A:391:GLY:H	1:A:394:ALA:HB3	1.83	0.43
1:A:431:LEU:O	1:A:438:PHE:CE2	2.70	0.43
1:A:616:TYR:C	1:A:618:GLY:H	2.26	0.43
1:A:627:ARG:C	1:A:629:GLY:N	2.75	0.43
1:A:477:GLY:O	1:A:479:PRO:HD3	2.18	0.43
1:A:519:ARG:HA	1:A:562:ASP:OD2	2.19	0.43
1:A:664:GLN:O	1:A:666:ARG:HG3	2.18	0.43
1:A:685:GLU:HA	1:A:688:ILE:CD1	2.49	0.43
1:A:215:LYS:O	1:A:218:GLU:HB3	2.19	0.43
1:A:443:HIS:HA	1:A:444:PRO:HD3	1.51	0.43
1:A:500:GLN:OE1	1:A:500:GLN:HA	2.19	0.43
1:A:631:ILE:HD12	1:A:631:ILE:H	1.83	0.43
1:A:27:THR:HG22	1:A:31:ARG:CG	2.48	0.43
1:A:671:MET:O	1:A:672:PHE:CD1	2.72	0.43
1:A:12:LEU:O	1:A:283:PRO:HD3	2.19	0.42
1:A:120:THR:O	1:A:123:ARG:HB2	2.18	0.42
1:A:251:ILE:HG23	1:A:281:PRO:HB3	2.01	0.42
1:A:350:GLU:OE1	1:A:380:LEU:HD23	2.19	0.42
1:A:493:VAL:CG2	1:A:593:ALA:HB2	2.41	0.42
1:A:21:ILE:HB	1:A:22:ASP:H	1.65	0.42
1:A:111:SER:OG	1:A:141:LYS:HD3	2.18	0.42
1:A:156:ARG:HH11	1:A:666:ARG:NH1	2.17	0.42
1:A:153:MET:HB3	1:A:153:MET:HE2	1.77	0.42
1:A:542:VAL:C	1:A:544:LYS:N	2.74	0.42
1:A:150:ILE:H	1:A:150:ILE:HG12	1.73	0.42
1:A:186:TYR:HE1	1:A:198:GLU:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ILE:HA	1:A:590:ILE:HD13	1.77	0.42
1:A:227:ILE:HD11	1:A:241:GLU:HB3	2.01	0.42
1:A:327:PHE:CE1	1:A:376:ALA:HB2	2.55	0.42
1:A:655:TYR:O	1:A:655:TYR:CD1	2.72	0.42
1:A:680:PRO:O	1:A:681:LYS:C	2.61	0.42
1:A:359:HIS:NE2	1:A:364:GLU:HB3	2.35	0.42
1:A:129:LYS:O	1:A:129:LYS:HD3	2.19	0.42
1:A:153:MET:CE	1:A:161:PRO:HB3	2.50	0.42
1:A:561:VAL:O	1:A:563:ILE:HG23	2.20	0.42
1:A:654:GLY:O	1:A:656:ALA:N	2.53	0.42
1:A:679:VAL:CG1	1:A:683:VAL:HB	2.46	0.42
1:A:38:ARG:HG3	1:A:39:ILE:H	1.85	0.42
1:A:94:VAL:O	1:A:95:GLU:C	2.62	0.42
1:A:181:LEU:HD12	1:A:181:LEU:C	2.45	0.42
1:A:354:ARG:CG	1:A:378:VAL:CG1	2.98	0.42
1:A:90:PHE:CD2	1:A:461:ILE:HD11	2.54	0.42
1:A:572:TYR:HD1	1:A:572:TYR:H	1.65	0.41
1:A:636:PRO:CA	1:A:641:GLN:HG2	2.48	0.41
1:A:5:VAL:CG2	1:A:6:GLU:H	2.29	0.41
1:A:484:ARG:HG2	1:A:676:TYR:HE2	1.85	0.41
1:A:606:MET:HE2	1:A:649:LEU:CD2	2.44	0.41
1:A:652:MET:HE3	1:A:655:TYR:CD2	2.56	0.41
1:A:31:ARG:NH2	1:A:266:ASN:HD21	2.18	0.41
1:A:674:ASP:OD2	1:A:675:HIS:ND1	2.53	0.41
1:A:647:VAL:HG11	1:A:652:MET:HE1	2.03	0.41
1:A:11:ARG:HD2	1:A:76:ASP:OD2	2.20	0.41
1:A:669:PHE:HD1	1:A:669:PHE:H	1.69	0.41
1:A:341:VAL:CG2	1:A:350:GLU:HB2	2.51	0.41
1:A:384:ILE:HB	1:A:385:THR:H	1.32	0.41
1:A:8:ASP:HB3	1:A:11:ARG:H	1.86	0.41
1:A:218:GLU:O	1:A:221:ALA:HB3	2.21	0.41
1:A:496:LYS:O	1:A:588:MET:HE1	2.21	0.41
1:A:624:LEU:CG	1:A:631:ILE:HD11	2.50	0.41
1:A:18:ALA:O	1:A:106:VAL:HA	2.21	0.41
1:A:69:VAL:HG12	1:A:69:VAL:O	2.19	0.41
1:A:165:GLN:HG3	1:A:260:LEU:CD1	2.48	0.41
1:A:230:LYS:HB3	1:A:235:GLU:O	2.20	0.41
1:A:467:LYS:O	1:A:468:ARG:NH1	2.54	0.41
1:A:612:THR:CG2	1:A:663:THR:HG21	2.51	0.41
1:A:617:MET:HE3	1:A:617:MET:HB3	1.53	0.41
1:A:579:GLU:C	1:A:581:ALA:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:HB3	1:A:380:LEU:CD2	2.51	0.40
1:A:443:HIS:HB2	1:A:450:ILE:CD1	2.51	0.40
1:A:166:LEU:HD22	1:A:180:VAL:HG11	2.03	0.40
1:A:531:GLY:O	1:A:532:GLY:O	2.40	0.40
1:A:627:ARG:HB3	1:A:647:VAL:CG2	2.52	0.40
1:A:87:HIS:CE1	1:A:90:PHE:CB	3.04	0.40
1:A:247:ARG:HD2	1:A:278:ASP:O	2.21	0.40
1:A:281:PRO:HA	1:A:285:ASP:OD2	2.21	0.40
1:A:296:GLY:O	1:A:297:GLU:CB	2.64	0.40
1:A:449:THR:O	1:A:450:ILE:CG2	2.69	0.40
1:A:655:TYR:O	1:A:656:ALA:C	2.61	0.40
1:A:319:ASP:OD2	1:A:363:ARG:NH2	2.51	0.40
1:A:499:ARG:NH1	1:A:499:ARG:CG	2.76	0.40
1:A:602:LEU:HD12	1:A:602:LEU:HA	1.97	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	620/691 (90%)	437 (70%)	115 (18%)	68 (11%)	0 1

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	69	VAL
1	A	82	ILE
1	A	104	ALA
1	A	138	LYS
1	A	174	PHE
1	A	233	GLU

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Mol	Chain	Res	Type
1	A	295	GLU
1	A	353	ALA
1	A	362	HIS
1	A	393	ASP
1	A	410	ASP
1	A	412	ALA
1	A	435	ASP
1	A	442	THR
1	A	443	HIS
1	A	454	MET
1	A	467	LYS
1	A	532	GLY
1	A	614	GLU
1	A	617	MET
1	A	649	LEU
1	A	652	MET
1	A	678	GLU
1	A	88	VAL
1	A	93	GLU
1	A	171	GLU
1	A	324	ARG
1	A	427	ALA
1	A	428	LEU
1	A	438	PHE
1	A	455	GLY
1	A	457	LEU
1	A	501	THR
1	A	536	LYS
1	A	555	LEU
1	A	639	ASN
1	A	662	LYS
1	A	6	GLU
1	A	23	ALA
1	A	137	ASN
1	A	140	ASP
1	A	144	ALA
1	A	348	ARG
1	A	368	GLU
1	A	384	ILE
1	A	415	PRO
1	A	468	ARG
1	A	640	ALA

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Mol	Chain	Res	Type
1	A	681	LYS
1	A	72	CYS
1	A	83	ASP
1	A	86	GLY
1	A	114	VAL
1	A	655	TYR
1	A	21	ILE
1	A	142	THR
1	A	478	LYS
1	A	580	MET
1	A	90	PHE
1	A	196	ILE
1	A	264	LEU
1	A	322	VAL
1	A	648	PRO
1	A	287	PRO
1	A	338	GLY
1	A	688	ILE
1	A	575	VAL

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	534/582 (92%)	396 (74%)	138 (26%)	0 2

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

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	TYR
1	A	11	ARG
1	A	12	LEU
1	A	15	ILE
1	A	27	THR
1	A	28	THR

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Mol	Chain	Res	Type
1	A	32	ILE
1	A	34	TYR
1	A	36	THR
1	A	38	ARG
1	A	39	ILE
1	A	83	ASP
1	A	84	THR
1	A	92	ILE
1	A	93	GLU
1	A	94	VAL
1	A	96	ARG
1	A	99	ARG
1	A	101	LEU
1	A	107	VAL
1	A	110	SER
1	A	115	GLU
1	A	118	SER
1	A	120	THR
1	A	123	ARG
1	A	129	LYS
1	A	131	PRO
1	A	137	ASN
1	A	151	ARG
1	A	156	ARG
1	A	157	LEU
1	A	166	LEU
1	A	175	SER
1	A	181	LEU
1	A	182	ARG
1	A	196	ILE
1	A	206	LEU
1	A	226	ASN
1	A	236	GLU
1	A	242	LEU
1	A	248	LYS
1	A	257	PRO
1	A	260	LEU
1	A	264	LEU
1	A	265	LYS
1	A	269	VAL
1	A	276	VAL
1	A	277	VAL

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Mol	Chain	Res	Type
1	A	278	ASP
1	A	288	PRO
1	A	293	THR
1	A	294	PRO
1	A	297	GLU
1	A	300	GLU
1	A	309	LEU
1	A	312	LEU
1	A	321	TYR
1	A	322	VAL
1	A	326	THR
1	A	329	ARG
1	A	335	LEU
1	A	337	SER
1	A	348	ARG
1	A	352	VAL
1	A	357	ARG
1	A	365	GLU
1	A	367	GLU
1	A	369	LEU
1	A	370	LYS
1	A	374	LEU
1	A	377	VAL
1	A	378	VAL
1	A	381	LYS
1	A	383	THR
1	A	384	ILE
1	A	389	LEU
1	A	396	ARG
1	A	398	ILE
1	A	413	ILE
1	A	414	GLU
1	A	415	PRO
1	A	435	ASP
1	A	437	THR
1	A	439	ARG
1	A	440	VAL
1	A	452	SER
1	A	458	HIS
1	A	464	ASP
1	A	466	LEU
1	A	468	ARG

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	484	ARG
1	A	492	ASP
1	A	506	GLN
1	A	514	VAL
1	A	517	LEU
1	A	518	PRO
1	A	519	ARG
1	A	533	VAL
1	A	537	GLU
1	A	540	PRO
1	A	550	MET
1	A	551	GLN
1	A	554	PRO
1	A	566	THR
1	A	572	TYR
1	A	574	GLU
1	A	575	VAL
1	A	579	GLU
1	A	580	MET
1	A	602	LEU
1	A	605	ILE
1	A	607	ARG
1	A	612	THR
1	A	614	GLU
1	A	619	ASP
1	A	621	ILE
1	A	623	ASP
1	A	625	ASN
1	A	632	LEU
1	A	634	MET
1	A	641	GLN
1	A	643	ILE
1	A	644	ARG
1	A	648	PRO
1	A	649	LEU
1	A	652	MET
1	A	657	THR
1	A	660	ARG
1	A	664	GLN
1	A	670	VAL
1	A	679	VAL

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Mol	Chain	Res	Type
1	A	681	LYS
1	A	682	GLN
1	A	683	VAL
1	A	686	LYS
1	A	689	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	80	ASN
1	A	87	HIS
1	A	208	GLN
1	A	266	ASN
1	A	302	HIS
1	A	343	ASN
1	A	426	GLN
1	A	595	GLN
1	A	625	ASN
1	A	664	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.