



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:58 PM UTC

PDB ID : 7XDR / pdb_00007xdr
Title : Crystal structure of a glucosylglycerol phosphorylase from *Marinobacter adhaerens*
Authors : Wei, H.L.; Li, Q.; Yang, J.G.; Liu, W.D.; Sun, Y.X.
Deposited on : 2022-03-28
Resolution : 2.40 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

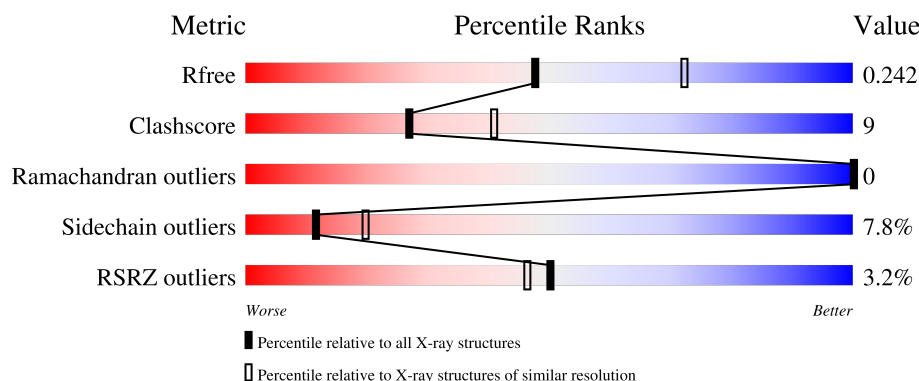
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

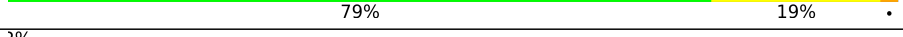
The reported resolution of this entry is 2.40 Å.

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.



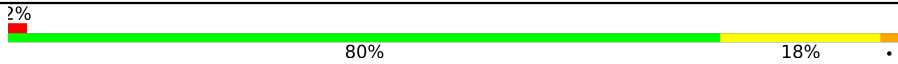
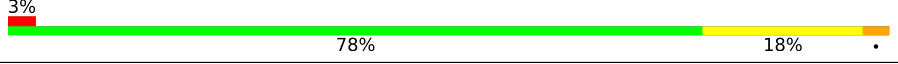
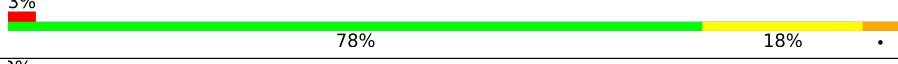
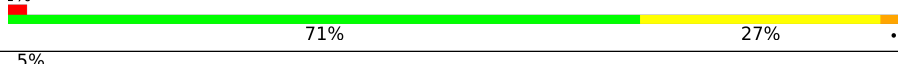
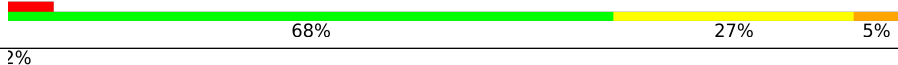
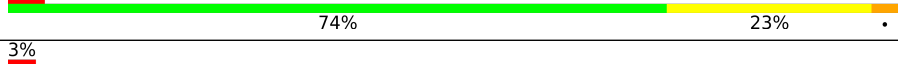
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	480	 82% 17% .
1	B	480	 80% 18% .
1	C	480	 82% 16% .
1	D	480	 79% 19% .
1	E	480	 82% 16% .

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Mol	Chain	Length	Quality of chain
1	F	480	
1	G	480	
1	H	480	
1	I	480	
1	J	480	
1	K	480	
1	L	480	
1	M	480	
1	N	480	
1	O	480	
1	P	480	
1	Q	480	
1	R	480	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 71196 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 Glucosylglycerol phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	B	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	C	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	D	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	E	479	Total	C	N	O	S	0	0	0
			3854	2459	638	736	21			
1	F	480	Total	C	N	O	S	0	0	0
			3850	2458	633	737	22			
1	G	479	Total	C	N	O	S	0	0	0
			3854	2459	638	736	21			
1	H	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	I	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	J	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	K	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	L	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	M	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	N	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	O	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	P	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			
1	R	480	Total	C	N	O	S	0	0	0
			3862	2464	639	737	22			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	163	Total	O	0	0
			163	163		
2	B	132	Total	O	0	0
			132	132		
2	C	148	Total	O	0	0
			148	148		
2	D	93	Total	O	0	0
			93	93		
2	E	146	Total	O	0	0
			146	146		
2	F	90	Total	O	0	0
			90	90		
2	G	104	Total	O	0	0
			104	104		
2	H	117	Total	O	0	0
			117	117		
2	I	83	Total	O	0	0
			83	83		
2	J	80	Total	O	0	0
			80	80		
2	K	101	Total	O	0	0
			101	101		
2	L	67	Total	O	0	0
			67	67		
2	M	74	Total	O	0	0
			74	74		
2	N	94	Total	O	0	0
			94	94		
2	O	46	Total	O	0	0
			46	46		
2	P	46	Total	O	0	0
			46	46		
2	Q	56	Total	O	0	0
			56	56		

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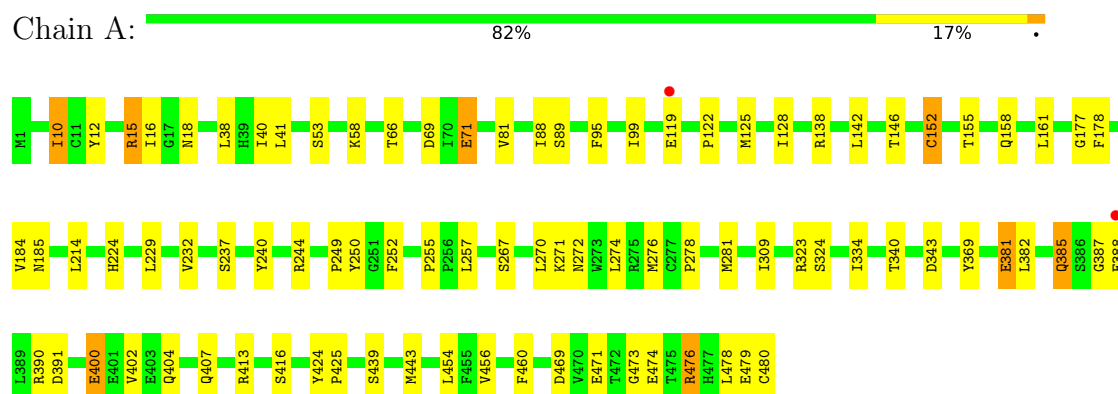
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	68	Total	O	0	0
			68	68		

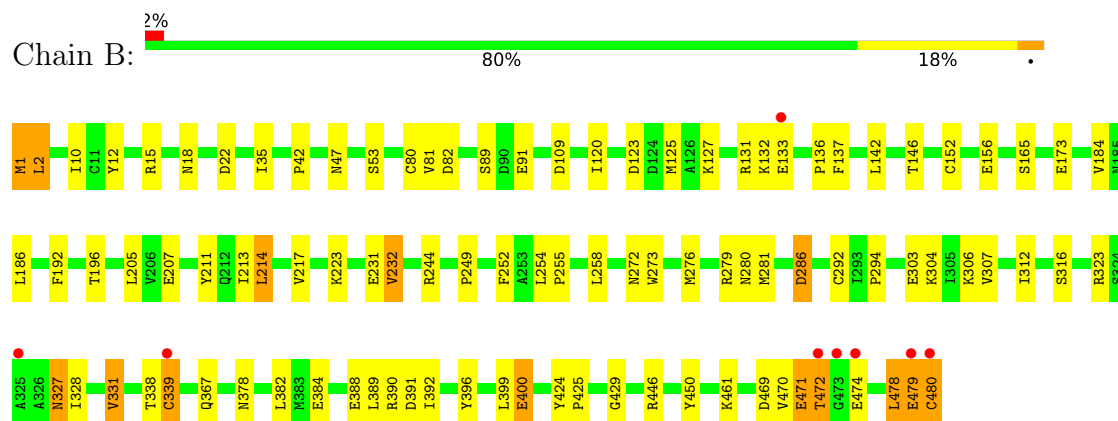
3 Residue-property plots

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

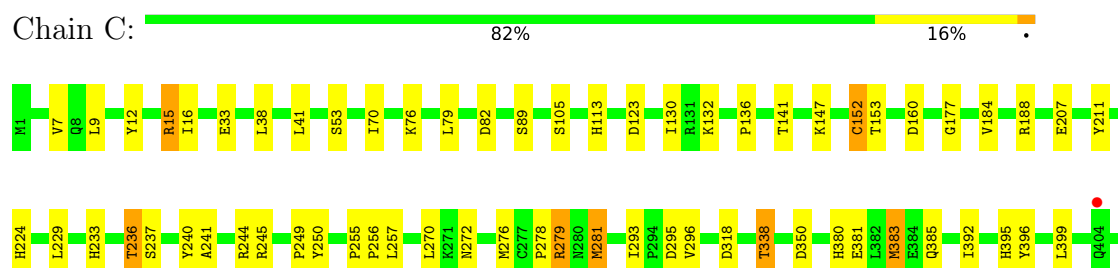
• Molecule 1: Glucosylglycerol phosphorylase



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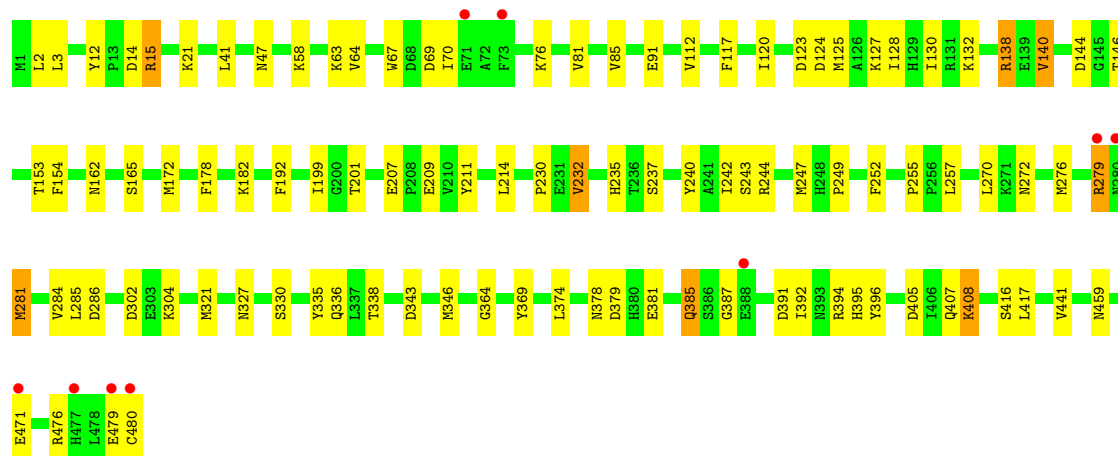
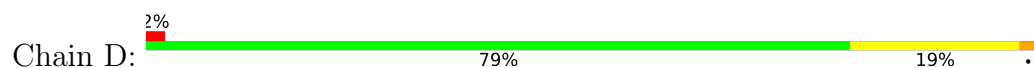


• Molecule 1: Glucosylglycerol phosphorylase

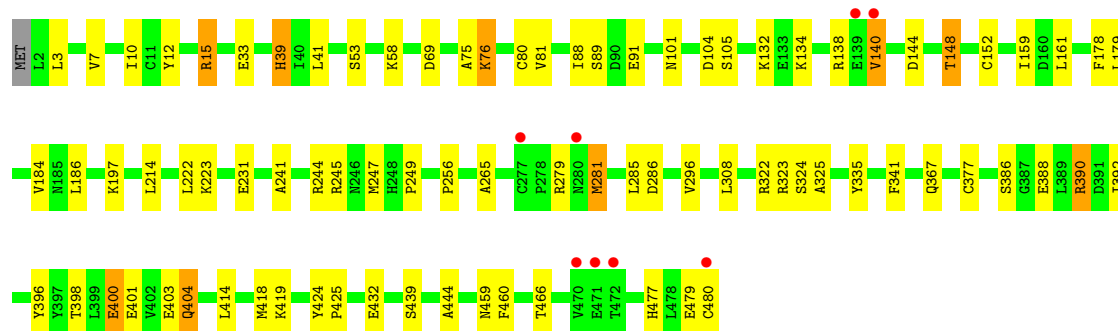
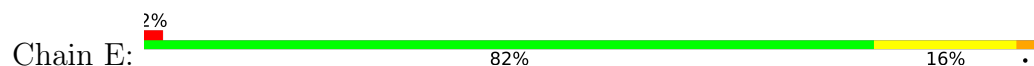




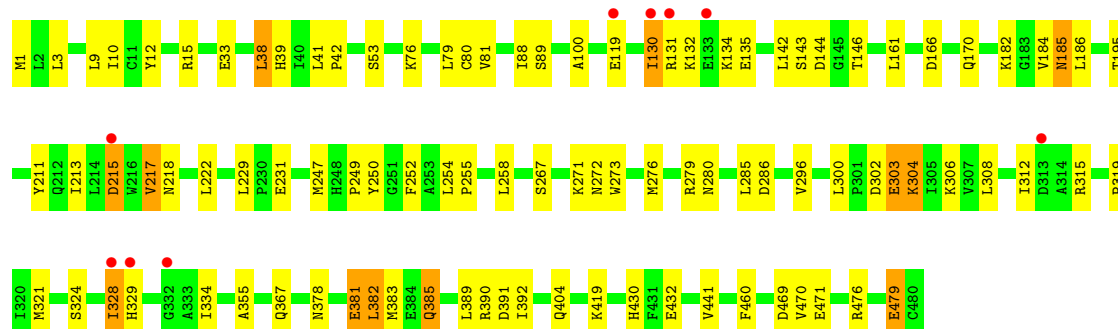
• Molecule 1: Glucosylglycerol phosphorylase



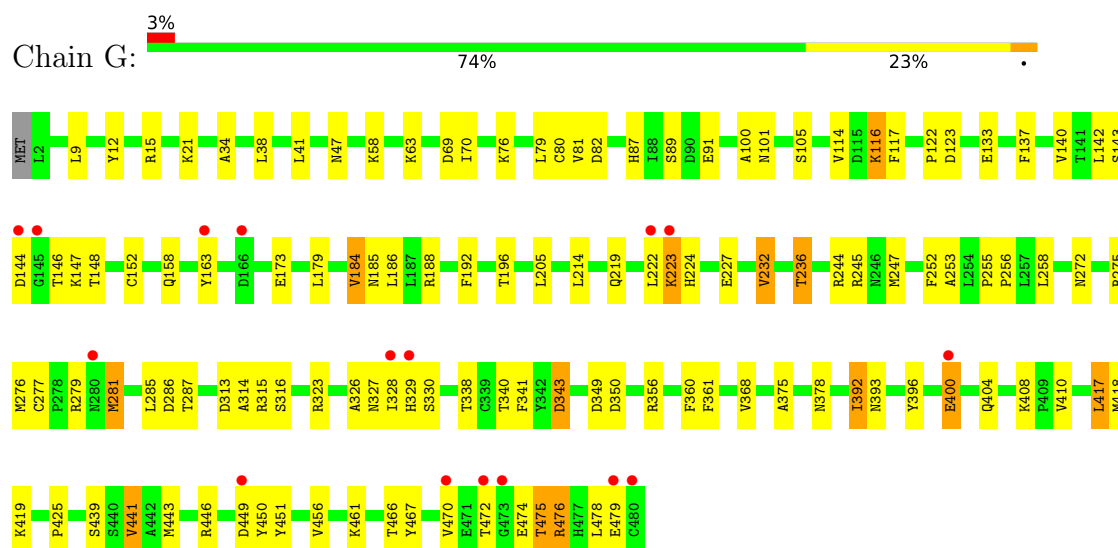
• Molecule 1: Glucosylglycerol phosphorylase



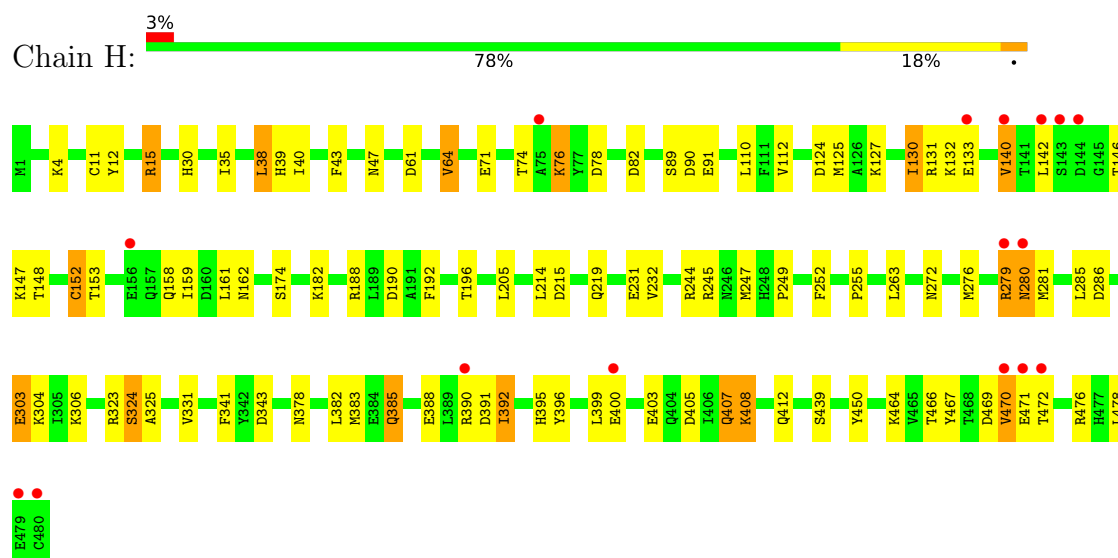
• Molecule 1: Glucosylglycerol phosphorylase



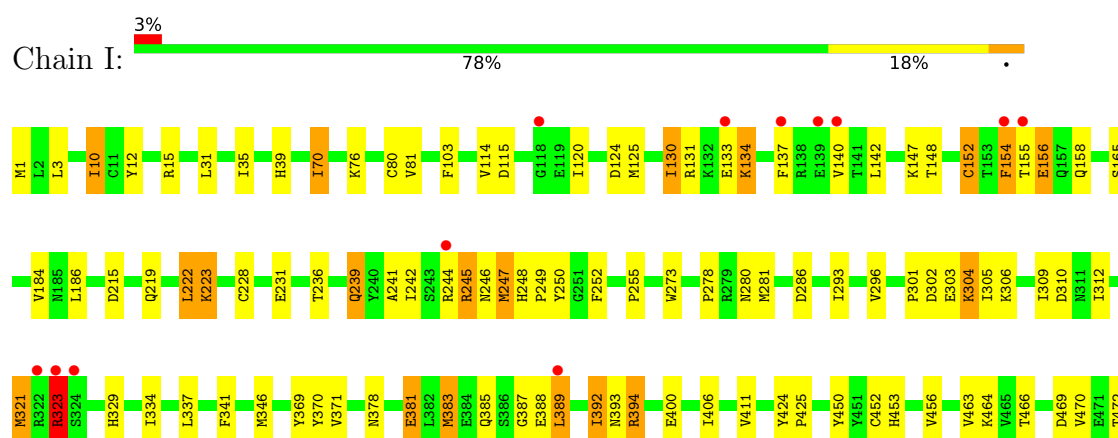
• Molecule 1: Glucosylglycerol phosphorylase

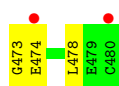


• Molecule 1: Glucosylglycerol phosphorylase

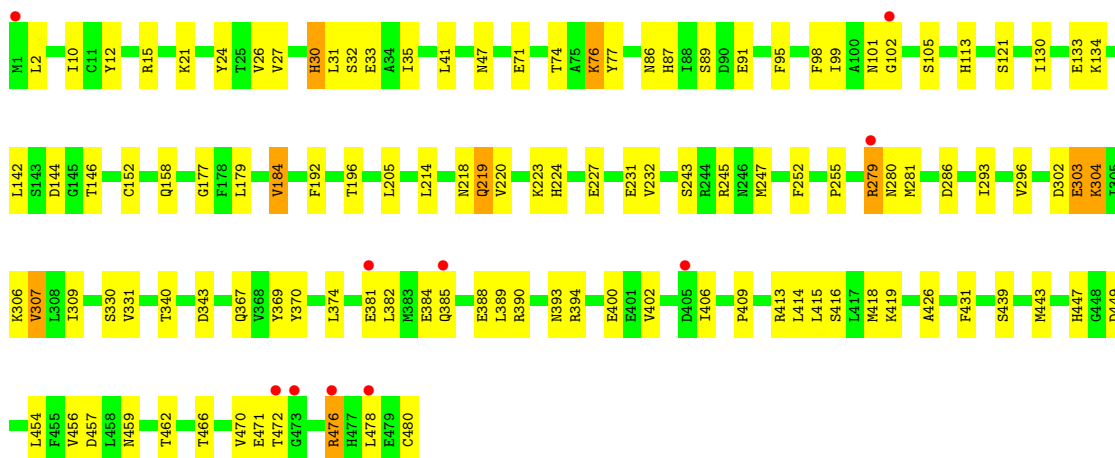
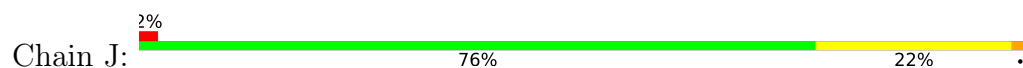


• Molecule 1: Glucosylglycerol phosphorylase

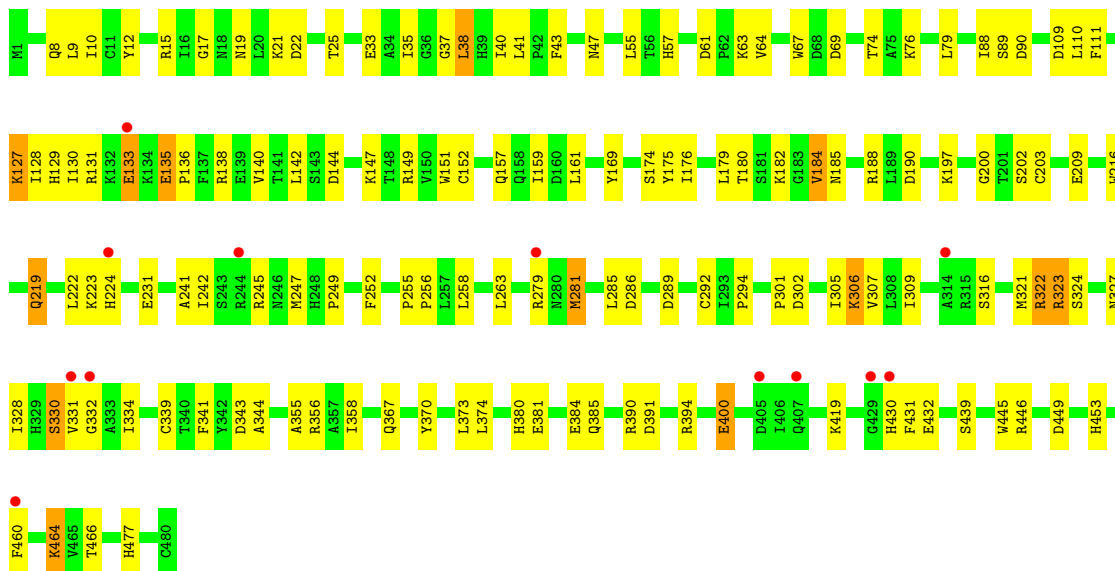




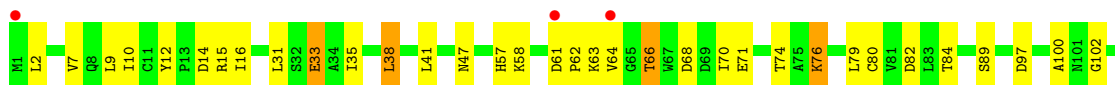
• Molecule 1: Glucosylglycerol phosphorylase

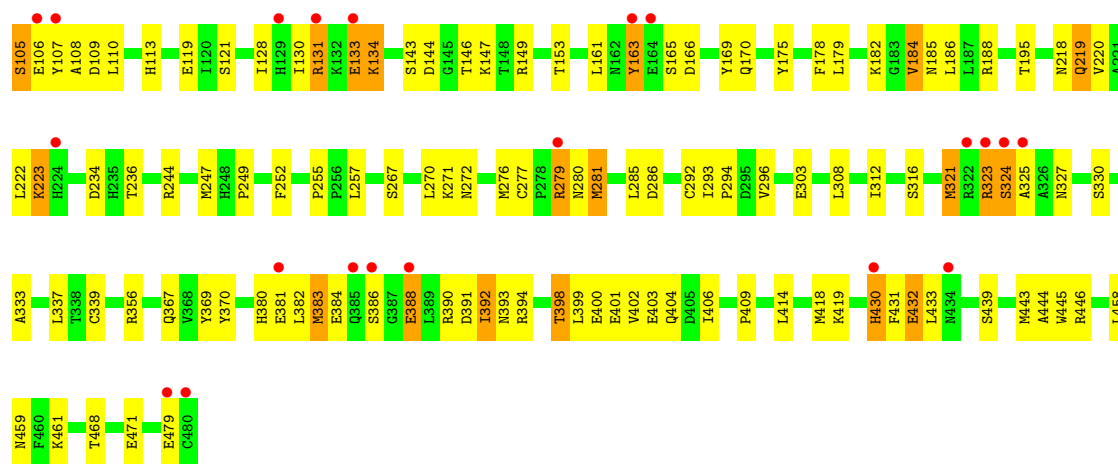


• Molecule 1: Glucosylglycerol phosphorylase

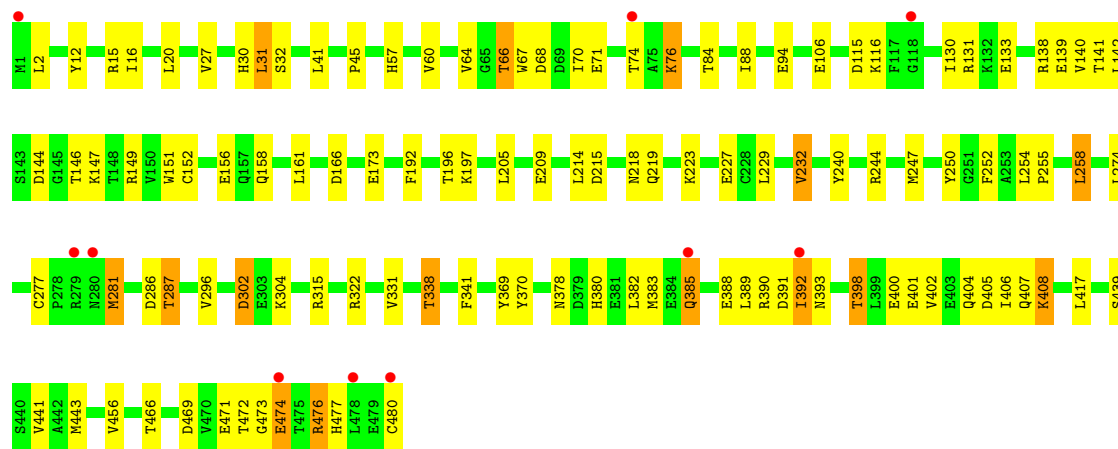
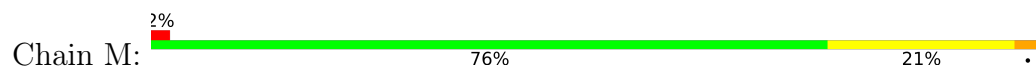


• Molecule 1: Glucosylglycerol phosphorylase

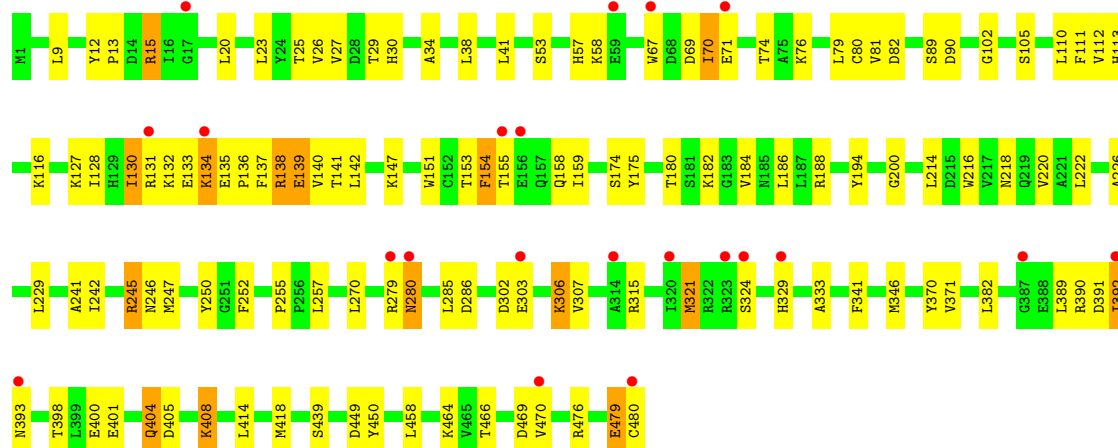
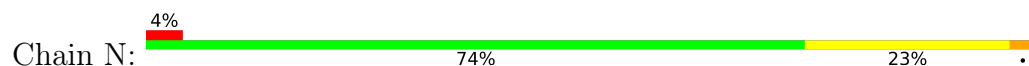




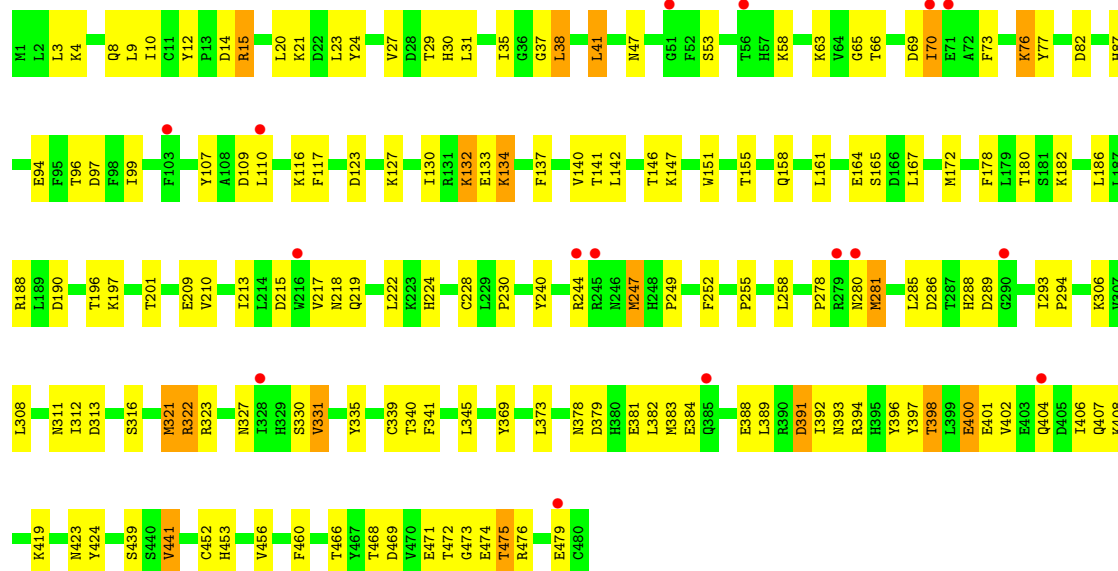
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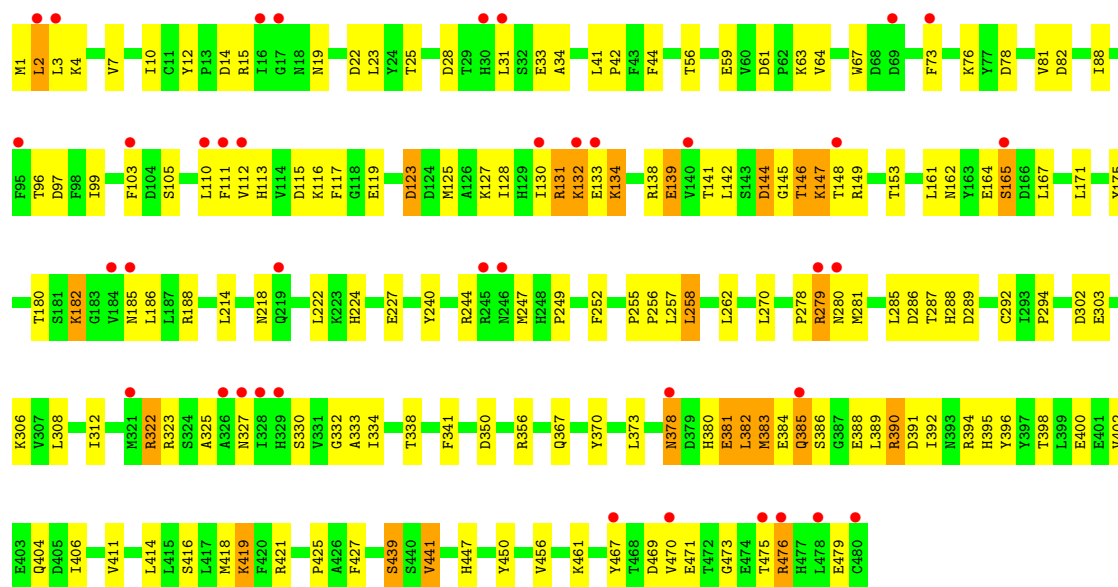
• Molecule 1: Glucosylglycerol phosphorylase



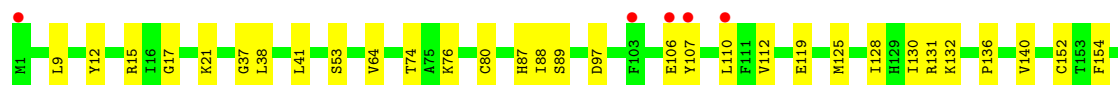
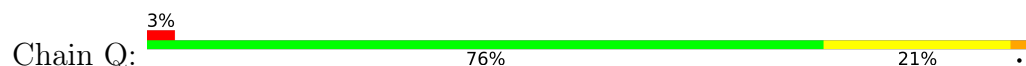
• Molecule 1: Glucosylglycerol phosphorylase

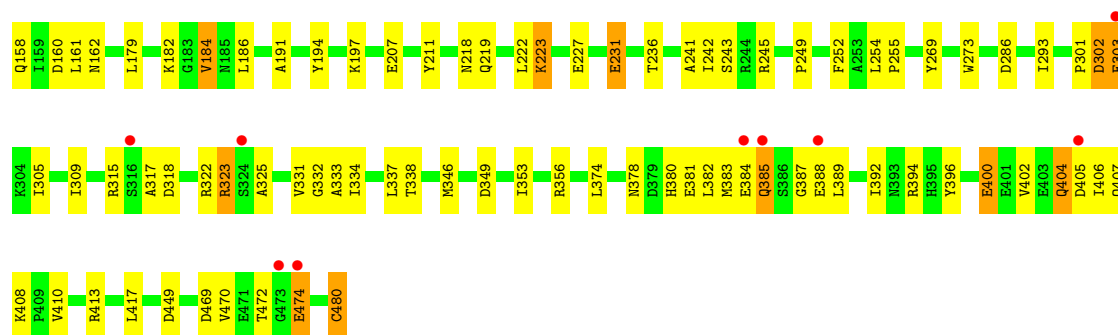


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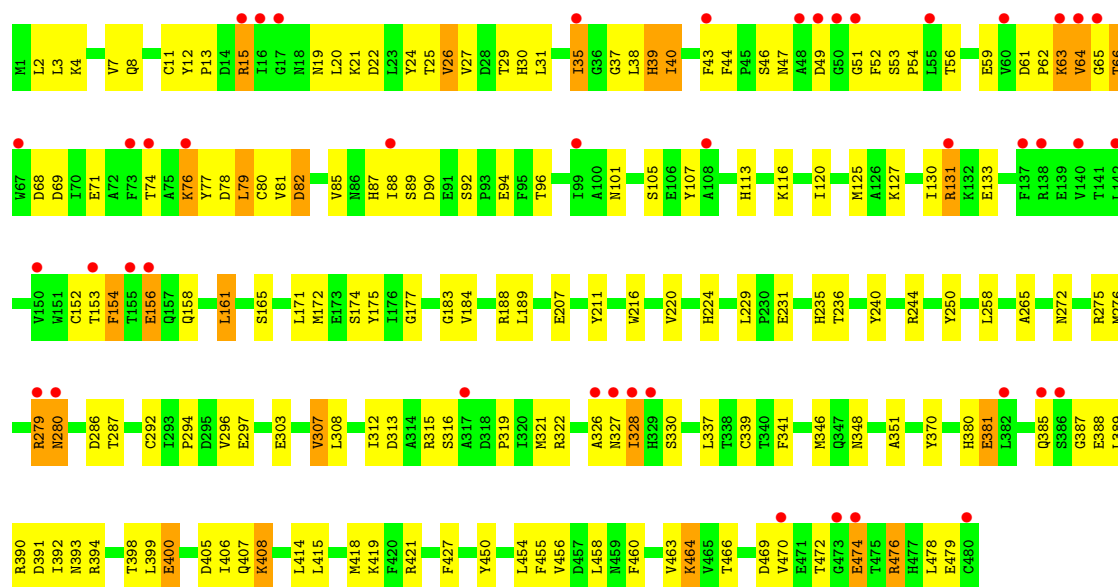


• Molecule 1: Glucosylglycerol phosphorylase





● Molecule 1: Glucosylglycerol phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.27Å 185.17Å 257.62Å 90.00° 101.56° 90.00°	Depositor
Resolution (Å)	33.40 – 2.40 33.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.40-2.40) 95.2 (33.40-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.237 0.206 , 0.242	Depositor DCC
R_{free} test set	18126 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	71196	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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	0.50	0/3959	0.72	3/5384 (0.1%)
1	B	0.49	0/3959	0.70	0/5384
1	C	0.49	0/3959	0.70	0/5384
1	D	0.48	0/3959	0.71	2/5384 (0.0%)
1	E	0.50	0/3951	0.72	0/5374
1	F	0.48	0/3947	0.70	2/5370 (0.0%)
1	G	0.52	0/3951	0.78	5/5374 (0.1%)
1	H	0.55	0/3959	0.77	1/5384 (0.0%)
1	I	0.53	0/3959	0.79	7/5384 (0.1%)
1	J	0.51	0/3959	0.75	1/5384 (0.0%)
1	K	0.60	0/3959	0.84	0/5384
1	L	0.54	0/3959	0.79	2/5384 (0.0%)
1	M	0.51	0/3959	0.75	0/5384
1	N	0.52	0/3959	0.78	4/5384 (0.1%)
1	O	0.51	0/3959	0.73	2/5384 (0.0%)
1	P	0.57	0/3959	0.83	1/5384 (0.0%)
1	Q	0.47	0/3959	0.69	3/5384 (0.1%)
1	R	0.60	0/3959	0.84	3/5384 (0.1%)
All	All	0.52	0/71234	0.76	36/96878 (0.0%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	470	VAL	CA-C-N	6.89	132.14	121.19
1	F	470	VAL	C-N-CA	6.89	132.14	121.19
1	P	164	GLU	N-CA-C	-6.88	103.23	111.69
1	L	324	SER	N-CA-C	-6.42	104.29	111.28
1	R	154	PHE	CB-CA-C	-6.27	109.35	116.63
1	N	246	ASN	CA-C-N	-6.23	112.81	122.59
1	N	246	ASN	C-N-CA	-6.23	112.81	122.59
1	I	387	GLY	N-CA-C	-6.09	106.84	115.30
1	Q	387	GLY	N-CA-C	-6.07	106.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	156	GLU	N-CA-C	-5.85	106.48	113.97
1	D	279	ARG	N-CA-C	5.80	117.28	111.07
1	H	147	LYS	CG-CD-CE	-5.76	98.04	111.30
1	G	196	THR	OG1-CB-CG2	5.76	120.81	109.30
1	I	278	PRO	CA-C-N	-5.73	112.50	122.64
1	I	278	PRO	C-N-CA	-5.73	112.50	122.64
1	I	147	LYS	CB-CG-CD	5.57	124.12	111.30
1	N	138	ARG	CA-C-N	5.57	128.74	120.95
1	N	138	ARG	C-N-CA	5.57	128.74	120.95
1	J	30	HIS	N-CA-C	5.56	117.42	111.36
1	O	4	LYS	CB-CA-C	-5.51	100.58	109.72
1	R	319	PRO	N-CA-C	5.49	120.11	111.38
1	R	387	GLY	N-CA-C	-5.46	107.73	115.43
1	A	71	GLU	N-CA-CB	5.45	119.58	110.32
1	D	387	GLY	N-CA-C	-5.38	107.82	115.30
1	A	122	PRO	N-CA-C	-5.28	106.19	113.53
1	Q	21	LYS	CG-CD-CE	5.23	123.34	111.30
1	G	163	TYR	CB-CA-C	5.17	120.19	110.63
1	G	326	ALA	CA-C-N	-5.15	116.15	122.84
1	G	326	ALA	C-N-CA	-5.15	116.15	122.84
1	G	122	PRO	N-CA-C	-5.11	106.43	113.53
1	I	323	ARG	CA-C-N	-5.04	116.28	123.03
1	I	323	ARG	C-N-CA	-5.04	116.28	123.03
1	A	387	GLY	N-CA-C	-5.04	108.33	115.43
1	O	4	LYS	N-CA-CB	5.03	117.42	109.83
1	L	163	TYR	CB-CA-C	5.03	119.14	110.79
1	Q	223	LYS	CB-CG-CD	-5.01	99.77	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3862	0	3724	48	0
1	B	3862	0	3724	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3862	0	3724	57	0
1	D	3862	0	3724	59	0
1	E	3854	0	3712	50	0
1	F	3850	0	3702	56	0
1	G	3854	0	3712	68	0
1	H	3862	0	3724	59	0
1	I	3862	0	3724	70	0
1	J	3862	0	3724	55	0
1	K	3862	0	3724	84	0
1	L	3862	0	3724	92	0
1	M	3862	0	3724	64	0
1	N	3862	0	3724	71	0
1	O	3862	0	3724	96	0
1	P	3862	0	3724	104	0
1	Q	3862	0	3724	70	0
1	R	3862	0	3724	118	0
2	A	163	0	0	1	0
2	B	132	0	0	2	0
2	C	148	0	0	5	0
2	D	93	0	0	3	0
2	E	146	0	0	6	0
2	F	90	0	0	3	0
2	G	104	0	0	5	0
2	H	117	0	0	3	0
2	I	83	0	0	3	0
2	J	80	0	0	1	0
2	K	101	0	0	3	0
2	L	67	0	0	3	0
2	M	74	0	0	1	0
2	N	94	0	0	1	0
2	O	46	0	0	2	0
2	P	46	0	0	3	0
2	Q	56	0	0	2	0
2	R	68	0	0	2	0
All	All	71196	0	66986	1249	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 9.

All (1249) 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:R:464:LYS:HE2	1:R:466:THR:HG23	1.48	0.95
1:F:329:HIS:HA	1:F:334:ILE:HD11	1.50	0.92
1:M:66:THR:HG22	1:M:68:ASP:H	1.34	0.91
1:L:218:ASN:HB2	1:L:247:MET:HE3	1.52	0.89
1:Q:472:THR:HG23	1:Q:474:GLU:H	1.38	0.89
1:J:12:TYR:HB2	1:J:15:ARG:HB2	1.54	0.89
1:P:287:THR:HG22	1:P:289:ASP:H	1.38	0.86
1:K:306:LYS:HD3	1:K:331:VAL:HG23	1.57	0.86
1:E:101:ASN:O	1:E:104:ASP:HB2	1.76	0.85
1:E:377:CYS:SG	2:E:575:HOH:O	2.34	0.85
1:C:472:THR:HG23	1:C:474:GLU:H	1.43	0.83
1:P:33:GLU:HB3	1:P:419:LYS:HD3	1.61	0.82
1:R:177:GLY:HA2	1:R:224:HIS:HD2	1.42	0.82
1:I:10:ILE:HG23	1:I:369:TYR:HA	1.59	0.81
1:P:78:ASP:HA	1:P:185:ASN:HD21	1.43	0.81
1:I:239:GLN:HG3	1:I:249:PRO:HB2	1.63	0.80
1:R:469:ASP:HB2	1:R:476:ARG:HD2	1.64	0.78
1:E:460:PHE:HA	1:K:133:GLU:O	1.83	0.78
1:F:479:GLU:OE1	1:F:479:GLU:N	2.17	0.77
1:F:211:TYR:O	1:F:215:ASP:HB2	1.84	0.77
1:I:371:VAL:HG21	1:I:393:ASN:O	1.83	0.77
1:J:47:ASN:HD22	1:J:91:GLU:HG3	1.47	0.77
1:B:327:ASN:HB2	1:R:307:VAL:HB	1.67	0.77
1:O:172:MET:HE3	1:O:172:MET:HA	1.67	0.77
1:I:450:TYR:HE1	1:I:470:VAL:HG13	1.49	0.77
1:C:12:TYR:HB2	1:C:15:ARG:HB2	1.67	0.76
1:P:391:ASP:HA	1:P:394:ARG:HB2	1.67	0.76
1:H:47:ASN:HD22	1:H:91:GLU:HG3	1.51	0.76
1:B:328:ILE:HD12	1:B:328:ILE:H	1.50	0.75
1:N:12:TYR:HB2	1:N:15:ARG:HB2	1.69	0.75
1:H:378:ASN:HB3	1:H:392:ILE:HD13	1.70	0.74
1:I:306:LYS:HE3	1:I:329:HIS:HB3	1.70	0.74
1:D:230:PRO:HG3	1:D:247:MET:HE2	1.68	0.73
1:P:303:GLU:HA	1:P:306:LYS:HD3	1.70	0.73
1:F:469:ASP:OD1	1:F:471:GLU:HB2	1.89	0.73
1:M:30:HIS:CD2	1:M:406:ILE:HG13	2.24	0.73
1:K:33:GLU:HB3	1:K:419:LYS:HG2	1.71	0.73
1:H:12:TYR:HB2	1:H:15:ARG:HB2	1.72	0.72
1:F:383:MET:HE3	1:F:392:ILE:HB	1.72	0.72
1:Q:130:ILE:HD13	1:Q:136:PRO:HG3	1.71	0.72
1:H:11:CYS:SG	1:H:38:LEU:HD21	2.30	0.72
1:I:301:PRO:HD2	1:I:304:LYS:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:371:VAL:HG21	1:N:393:ASN:O	1.90	0.72
1:O:10:ILE:HG23	1:O:369:TYR:HA	1.71	0.72
1:B:142:LEU:HD12	1:B:146:THR:HB	1.71	0.71
1:Q:469:ASP:HB3	1:Q:472:THR:HG22	1.71	0.71
1:J:449:ASP:HB3	1:J:470:VAL:HG22	1.71	0.71
1:N:82:ASP:OD2	1:N:188:ARG:NH1	2.23	0.71
1:H:324:SER:OG	1:H:325:ALA:N	2.19	0.70
1:N:450:TYR:HE1	1:N:470:VAL:HG13	1.56	0.70
1:A:400:GLU:HG3	1:A:404:GLN:HE22	1.57	0.70
1:C:241:ALA:O	1:C:245:ARG:HG2	1.92	0.70
1:G:314:ALA:HB2	2:G:505:HOH:O	1.91	0.70
1:L:391:ASP:HA	1:L:394:ARG:HB2	1.74	0.70
1:J:459:ASN:HB3	1:O:323:ARG:HH21	1.56	0.69
1:K:460:PHE:HE1	1:L:130:ILE:HD11	1.58	0.69
1:D:12:TYR:HB2	1:D:15:ARG:HB2	1.73	0.69
1:L:414:LEU:O	1:L:418:MET:HG3	1.92	0.69
1:I:114:VAL:HG21	1:I:137:PHE:HB3	1.74	0.69
1:J:144:ASP:OD1	1:J:146:THR:HG22	1.92	0.69
1:F:9:LEU:HD23	1:F:38:LEU:HD11	1.75	0.69
1:H:249:PRO:HD2	1:H:280:ASN:O	1.93	0.69
1:P:218:ASN:HB2	1:P:247:MET:HE3	1.74	0.68
1:P:67:TRP:CZ3	1:P:182:LYS:HG3	2.29	0.68
1:M:405:ASP:HA	1:M:408:LYS:HD3	1.75	0.68
1:H:245:ARG:HG3	1:H:245:ARG:HH11	1.59	0.68
1:I:453:HIS:ND1	2:I:503:HOH:O	2.27	0.67
1:A:38:LEU:CD2	1:A:40:ILE:HG12	2.24	0.67
1:E:15:ARG:HD2	1:E:396:TYR:CE2	2.29	0.67
1:G:12:TYR:HB2	1:G:15:ARG:HG2	1.74	0.67
1:E:244:ARG:HG2	1:E:244:ARG:HH11	1.59	0.67
1:G:400:GLU:HG3	1:L:409:PRO:HG2	1.76	0.67
1:L:380:HIS:O	1:L:384:GLU:HG2	1.95	0.67
1:R:46:SER:HB3	1:R:51:GLY:HA2	1.77	0.67
1:D:21:LYS:HE3	1:D:69:ASP:OD1	1.96	0.66
1:H:279:ARG:HG2	1:H:280:ASN:N	2.10	0.66
1:P:12:TYR:HB2	1:P:15:ARG:HB2	1.75	0.66
1:L:110:LEU:HD11	1:L:161:LEU:HD22	1.78	0.66
1:F:218:ASN:HB2	1:F:247:MET:HE3	1.77	0.66
1:M:30:HIS:HD2	1:M:406:ILE:HG13	1.60	0.66
1:R:15:ARG:HG3	1:R:370:TYR:OH	1.96	0.66
1:N:252:PHE:O	1:N:255:PRO:HD2	1.95	0.66
1:B:132:LYS:HE3	1:B:136:PRO:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:450:TYR:CE1	1:I:470:VAL:HG13	2.30	0.66
1:I:309:ILE:HG21	1:I:334:ILE:HD12	1.77	0.65
1:B:47:ASN:HD22	1:B:91:GLU:HG3	1.62	0.65
1:F:12:TYR:HB2	1:F:15:ARG:HB2	1.77	0.65
1:R:464:LYS:HE2	1:R:466:THR:CG2	2.23	0.65
1:O:141:THR:HG22	1:O:147:LYS:HG2	1.77	0.65
1:O:382:LEU:HD11	1:O:396:TYR:HD1	1.61	0.65
1:A:38:LEU:HD23	1:A:40:ILE:HG12	1.78	0.65
1:D:124:ASP:HA	1:D:127:LYS:HD2	1.79	0.65
1:C:9:LEU:HD23	1:C:38:LEU:HD11	1.79	0.65
1:K:10:ILE:HD11	1:K:367:GLN:HB3	1.78	0.64
1:G:142:LEU:HD12	1:G:146:THR:HB	1.79	0.64
1:L:131:ARG:CZ	1:L:131:ARG:H	2.09	0.64
1:Q:53:SER:HB2	1:Q:158:GLN:HG3	1.78	0.64
1:D:405:ASP:HA	1:D:408:LYS:HD3	1.80	0.64
1:I:389:LEU:O	1:I:392:ILE:HG22	1.97	0.64
1:O:378:ASN:HB3	1:O:392:ILE:HD11	1.78	0.64
1:R:76:LYS:HD3	1:R:77:TYR:CE1	2.32	0.64
1:Q:252:PHE:O	1:Q:255:PRO:HD2	1.97	0.64
1:N:127:LYS:NZ	1:N:200:GLY:O	2.24	0.64
1:A:10:ILE:HG12	1:A:369:TYR:HD1	1.63	0.64
1:L:14:ASP:OD1	1:L:14:ASP:N	2.30	0.63
1:R:20:LEU:HD12	1:R:65:GLY:HA3	1.80	0.63
1:O:398:THR:OG1	1:O:400:GLU:HG2	1.98	0.63
1:O:419:LYS:O	1:O:423:ASN:ND2	2.28	0.63
1:E:3:LEU:HD11	1:E:186:LEU:HD13	1.81	0.63
1:L:66:THR:HG23	1:L:68:ASP:H	1.64	0.63
1:R:11:CYS:SG	1:R:38:LEU:HD21	2.38	0.63
1:R:12:TYR:HB2	1:R:15:ARG:HB2	1.79	0.63
1:A:460:PHE:HE1	1:C:130:ILE:HD11	1.64	0.63
1:N:141:THR:OG1	1:N:147:LYS:NZ	2.30	0.63
1:C:469:ASP:HB3	1:C:472:THR:HG22	1.81	0.63
1:F:33:GLU:OE2	1:F:419:LYS:NZ	2.26	0.62
1:A:240:TYR:CZ	1:A:278:PRO:HD3	2.35	0.62
1:O:466:THR:HG23	1:O:475:THR:HG23	1.80	0.62
1:R:12:TYR:HB2	1:R:15:ARG:HG2	1.80	0.62
1:R:405:ASP:HA	1:R:408:LYS:HD3	1.80	0.62
1:B:286:ASP:OD1	1:B:286:ASP:N	2.29	0.62
1:D:63:LYS:HD3	1:O:63:LYS:HE2	1.81	0.62
1:K:47:ASN:ND2	1:K:89:SER:OG	2.25	0.62
1:O:142:LEU:HD12	1:O:146:THR:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:97:ASP:HB3	1:L:107:TYR:HD2	1.65	0.62
1:R:21:LYS:O	1:R:25:THR:HG23	2.00	0.62
1:B:120:ILE:HG21	1:B:125:MET:HE2	1.80	0.62
1:L:292:CYS:SG	1:L:294:PRO:HD2	2.39	0.62
1:B:378:ASN:HB3	1:B:392:ILE:HD11	1.82	0.61
1:L:316:SER:HB2	1:L:339:CYS:HB3	1.82	0.61
1:N:138:ARG:HE	1:N:140:VAL:HG12	1.63	0.61
1:K:258:LEU:HD12	1:K:285:LEU:HD11	1.81	0.61
1:P:382:LEU:HD11	1:P:396:TYR:HD1	1.65	0.61
1:L:325:ALA:HB1	1:L:333:ALA:HA	1.83	0.61
1:G:313:ASP:OD2	1:G:314:ALA:N	2.34	0.61
1:E:323:ARG:NH2	2:E:506:HOH:O	2.32	0.61
1:F:460:PHE:HE1	1:J:130:ILE:HD11	1.66	0.61
1:K:309:ILE:HG21	1:K:334:ILE:HD13	1.82	0.61
1:P:31:LEU:HD21	1:P:373:LEU:HD21	1.83	0.61
1:I:131:ARG:O	1:I:323:ARG:HB3	2.00	0.61
1:O:209:GLU:OE2	1:O:209:GLU:N	2.28	0.61
1:P:244:ARG:HA	1:P:279:ARG:HH22	1.66	0.61
1:P:322:ARG:NH1	1:P:332:GLY:O	2.33	0.61
1:B:389:LEU:O	1:B:392:ILE:HG22	2.01	0.61
1:H:38:LEU:HD22	1:H:40:ILE:HG13	1.82	0.60
1:I:15:ARG:HG2	1:I:370:TYR:OH	2.00	0.60
1:D:192:PHE:CE1	1:D:232:VAL:HG22	2.35	0.60
1:P:338:THR:HG21	1:P:389:LEU:HB3	1.81	0.60
1:R:177:GLY:HA2	1:R:224:HIS:CD2	2.32	0.60
1:E:12:TYR:HB2	1:E:15:ARG:HB2	1.81	0.60
1:R:303:GLU:O	1:R:307:VAL:HG13	2.02	0.60
1:J:47:ASN:ND2	1:J:91:GLU:HG3	2.15	0.60
1:C:472:THR:HG23	1:C:474:GLU:N	2.12	0.60
1:H:405:ASP:HA	1:H:408:LYS:HD3	1.83	0.60
1:L:219:GLN:HE22	1:L:223:LYS:HZ2	1.48	0.60
1:N:464:LYS:NZ	2:N:506:HOH:O	2.35	0.60
1:N:102:GLY:HA2	1:N:142:LEU:HD22	1.82	0.60
1:L:47:ASN:ND2	1:L:89:SER:OG	2.35	0.60
1:I:12:TYR:HB2	1:I:15:ARG:HB2	1.84	0.59
1:M:338:THR:HG21	1:M:389:LEU:HB3	1.83	0.59
1:P:110:LEU:HD11	1:P:161:LEU:HD22	1.84	0.59
1:J:457:ASP:HB3	1:J:462:THR:HG22	1.84	0.59
1:L:7:VAL:HG11	1:L:418:MET:HE3	1.83	0.59
1:N:414:LEU:O	1:N:418:MET:HG3	2.03	0.59
1:D:15:ARG:HD2	1:D:396:TYR:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ASN:HD22	1:D:91:GLU:HG3	1.68	0.59
1:K:286:ASP:OD1	1:K:356:ARG:NH2	2.35	0.59
1:I:472:THR:OG1	1:I:474:GLU:HG2	2.03	0.59
1:M:240:TYR:O	1:M:244:ARG:HD3	2.03	0.59
1:E:459:ASN:HB3	1:K:323:ARG:HH11	1.66	0.59
1:J:220:VAL:HA	1:J:223:LYS:HE2	1.85	0.59
1:M:27:VAL:HA	1:M:31:LEU:HD12	1.84	0.59
1:A:138:ARG:NE	2:A:509:HOH:O	2.35	0.59
1:F:9:LEU:HB3	1:F:38:LEU:HD12	1.83	0.59
1:J:303:GLU:O	1:J:307:VAL:HG13	2.02	0.59
1:P:78:ASP:HA	1:P:185:ASN:ND2	2.17	0.59
1:K:142:LEU:HB2	1:K:144:ASP:OD1	2.03	0.58
1:K:316:SER:HB2	1:K:339:CYS:HB3	1.85	0.58
1:O:252:PHE:O	1:O:255:PRO:HD2	2.03	0.58
1:I:152:CYS:SG	1:I:155:THR:O	2.61	0.58
1:N:80:CYS:HB2	1:N:186:LEU:HB3	1.85	0.58
1:O:383:MET:HE3	1:O:392:ILE:HB	1.85	0.58
1:C:257:LEU:HD21	1:C:270:LEU:HA	1.85	0.58
1:K:79:LEU:HD23	1:K:184:VAL:HG12	1.85	0.58
1:P:447:HIS:ND1	2:P:502:HOH:O	2.26	0.58
1:D:47:ASN:ND2	1:D:91:GLU:HG3	2.19	0.58
1:J:152:CYS:HB2	1:J:158:GLN:O	2.04	0.58
1:A:12:TYR:HB2	1:A:15:ARG:HB2	1.85	0.58
1:C:113:HIS:ND1	2:C:504:HOH:O	2.32	0.58
1:I:249:PRO:HD2	1:I:280:ASN:O	2.04	0.58
1:K:328:ILE:O	1:K:334:ILE:HD11	2.03	0.58
1:E:101:ASN:HB2	1:E:105:SER:HB2	1.86	0.58
1:L:195:THR:HA	2:L:502:HOH:O	2.03	0.58
1:B:303:GLU:HA	1:B:306:LYS:HD2	1.85	0.58
1:D:214:LEU:HG	1:D:247:MET:HE1	1.85	0.58
1:L:325:ALA:HB1	1:L:333:ALA:CB	2.34	0.58
1:A:257:LEU:HD21	1:A:270:LEU:HA	1.86	0.58
1:M:12:TYR:HB2	1:M:15:ARG:HB2	1.85	0.58
1:E:460:PHE:HE1	1:K:130:ILE:HD11	1.68	0.57
1:C:318:ASP:O	1:C:338:THR:OG1	2.22	0.57
1:M:152:CYS:HB2	1:M:158:GLN:O	2.04	0.57
1:M:205:LEU:HD21	1:M:232:VAL:HG11	1.86	0.57
1:N:13:PRO:HB3	1:N:20:LEU:HD21	1.86	0.57
1:O:9:LEU:HD23	1:O:38:LEU:HD11	1.86	0.57
1:O:188:ARG:NH1	1:O:190:ASP:OD1	2.37	0.57
1:R:279:ARG:HH11	1:R:280:ASN:HD21	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:HE1	1:B:137:PHE:HZ	1.68	0.57
1:F:319:PRO:HG2	1:F:321:MET:CE	2.35	0.57
1:Q:353:ILE:HG23	1:Q:417:LEU:HD11	1.85	0.57
1:P:125:MET:HA	1:P:128:ILE:HD12	1.86	0.57
1:Q:472:THR:HG23	1:Q:474:GLU:N	2.15	0.57
1:G:467:TYR:CZ	1:G:476:ARG:HB2	2.40	0.57
1:L:57:HIS:HB2	1:L:175:TYR:CD1	2.40	0.57
1:L:323:ARG:HD3	1:L:324:SER:H	1.69	0.57
1:M:378:ASN:HB3	1:M:392:ILE:HG23	1.86	0.57
1:O:12:TYR:HB2	1:O:15:ARG:HB2	1.87	0.57
1:M:141:THR:CG2	1:M:147:LYS:HE2	2.34	0.57
1:N:405:ASP:HA	1:N:408:LYS:HD3	1.85	0.57
1:K:252:PHE:O	1:K:255:PRO:HD2	2.04	0.57
1:R:24:TYR:OH	1:R:76:LYS:HD2	2.03	0.57
1:R:40:ILE:HB	1:R:43:PHE:HE2	1.70	0.57
1:I:312:ILE:HG21	1:I:337:LEU:HD13	1.87	0.57
1:F:166:ASP:O	1:F:170:GLN:HG3	2.05	0.56
1:L:219:GLN:O	1:L:223:LYS:HG2	2.05	0.56
1:O:53:SER:HB2	1:O:158:GLN:HG3	1.87	0.56
1:C:33:GLU:HB2	1:C:419:LYS:HD3	1.87	0.56
1:H:140:VAL:HG22	1:H:148:THR:HG22	1.86	0.56
1:L:12:TYR:HB2	1:L:15:ARG:HG2	1.85	0.56
1:P:402:VAL:O	1:P:406:ILE:HG12	2.04	0.56
1:Q:131:ARG:HB2	1:Q:131:ARG:CZ	2.35	0.56
1:R:286:ASP:OD1	1:R:286:ASP:N	2.37	0.56
1:G:179:LEU:O	1:G:184:VAL:HG13	2.06	0.56
1:P:286:ASP:OD1	1:P:286:ASP:N	2.30	0.56
1:L:398:THR:HG23	1:L:401:GLU:HB2	1.87	0.56
1:M:472:THR:HG22	1:M:474:GLU:HB3	1.87	0.56
1:P:131:ARG:O	1:P:323:ARG:HB2	2.06	0.56
1:Q:405:ASP:HA	1:Q:408:LYS:HD3	1.87	0.56
1:B:173:GLU:OE2	1:B:223:LYS:NZ	2.36	0.56
1:D:192:PHE:HE1	1:D:232:VAL:HG22	1.70	0.56
1:E:265:ALA:CB	1:K:324:SER:HB2	2.36	0.56
1:G:152:CYS:HB2	1:G:158:GLN:O	2.06	0.56
1:O:249:PRO:HD2	1:O:281:MET:HA	1.87	0.56
1:D:58:LYS:HG2	1:D:178:PHE:CG	2.40	0.56
1:N:382:LEU:HD23	1:N:391:ASP:HB3	1.88	0.56
1:C:467:TYR:CE2	1:C:476:ARG:HG3	2.41	0.56
1:B:478:LEU:HD13	1:B:480:CYS:H	1.70	0.56
1:P:257:LEU:HD21	1:P:270:LEU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:ASP:O	1:L:64:VAL:HG22	2.06	0.56
1:B:125:MET:HE1	1:B:137:PHE:CZ	2.41	0.55
1:G:476:ARG:CZ	1:G:476:ARG:HB3	2.35	0.55
1:H:43:PHE:HB2	1:H:64:VAL:HG21	1.87	0.55
1:H:450:TYR:HE1	1:H:470:VAL:HB	1.71	0.55
1:R:53:SER:HB2	1:R:158:GLN:HG3	1.87	0.55
1:E:214:LEU:HB3	1:E:247:MET:HE1	1.88	0.55
1:K:57:HIS:HB2	1:K:175:TYR:CD1	2.40	0.55
1:P:414:LEU:O	1:P:418:MET:HG3	2.06	0.55
1:Q:219:GLN:O	1:Q:223:LYS:HD2	2.06	0.55
1:R:15:ARG:HG3	1:R:370:TYR:CZ	2.41	0.55
1:A:229:LEU:HD21	1:A:250:TYR:CZ	2.41	0.55
1:F:382:LEU:O	1:F:385:GLN:HG3	2.06	0.55
1:O:178:PHE:O	1:O:182:LYS:HG2	2.07	0.55
1:P:249:PRO:HD2	1:P:281:MET:HA	1.87	0.55
1:K:12:TYR:HB2	1:K:15:ARG:HB2	1.89	0.55
1:B:252:PHE:O	1:B:255:PRO:HD2	2.06	0.55
1:G:277:CYS:HB2	1:G:281:MET:HE1	1.88	0.55
1:G:340:THR:OG1	1:G:343:ASP:HB2	2.07	0.55
1:N:128:ILE:HG22	1:N:130:ILE:HG12	1.89	0.55
1:K:431:PHE:HB2	1:K:445:TRP:CH2	2.41	0.55
1:P:294:PRO:HG3	1:P:322:ARG:NH2	2.22	0.55
1:Q:125:MET:HA	1:Q:128:ILE:HD12	1.87	0.55
1:Q:381:GLU:HG2	1:Q:385:GLN:HE21	1.71	0.55
1:B:47:ASN:ND2	1:B:91:GLU:HG3	2.21	0.55
1:A:152:CYS:HB2	1:A:158:GLN:O	2.06	0.55
1:C:229:LEU:HD21	1:C:250:TYR:CZ	2.41	0.55
1:D:391:ASP:HA	1:D:394:ARG:HB2	1.89	0.55
1:G:116:LYS:HG2	1:G:117:PHE:N	2.21	0.55
1:H:90:ASP:HB3	1:H:159:ILE:HD11	1.89	0.55
1:R:94:GLU:HA	1:R:107:TYR:CD1	2.42	0.55
1:F:303:GLU:HG3	1:F:304:LYS:N	2.21	0.55
1:I:155:THR:HG22	1:I:156:GLU:H	1.71	0.55
1:O:382:LEU:HD11	1:O:396:TYR:CD1	2.42	0.55
1:I:378:ASN:HB3	1:I:392:ILE:HG13	1.88	0.55
1:K:19:ASN:ND2	2:K:504:HOH:O	2.35	0.55
1:L:9:LEU:HD23	1:L:38:LEU:HD21	1.89	0.55
1:P:144:ASP:CG	1:P:146:THR:H	2.15	0.55
1:O:180:THR:HG21	1:O:224:HIS:HB3	1.88	0.54
1:O:306:LYS:HE2	1:O:331:VAL:HG13	1.89	0.54
1:C:7:VAL:HG11	1:C:418:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:TYR:OH	1:J:76:LYS:HD3	2.07	0.54
1:O:286:ASP:OD1	1:O:286:ASP:N	2.40	0.54
1:F:195:THR:HA	2:F:504:HOH:O	2.08	0.54
1:G:205:LEU:HD21	1:G:232:VAL:HG11	1.89	0.54
1:J:142:LEU:HD12	1:J:146:THR:HG23	1.89	0.54
1:J:286:ASP:CG	1:J:369:TYR:HB3	2.32	0.54
1:K:200:GLY:N	2:K:506:HOH:O	2.39	0.54
1:K:327:ASN:HB3	1:K:330:SER:HB3	1.88	0.54
1:P:82:ASP:OD2	1:P:188:ARG:NH1	2.40	0.54
1:A:252:PHE:O	1:A:255:PRO:HD2	2.07	0.54
1:N:321:MET:HE1	1:N:333:ALA:HB1	1.90	0.54
1:E:400:GLU:O	1:E:404:GLN:HG3	2.08	0.54
1:Q:469:ASP:HB3	1:Q:472:THR:CG2	2.37	0.54
1:K:249:PRO:HD2	1:K:281:MET:HA	1.89	0.54
1:O:94:GLU:HA	1:O:107:TYR:CD2	2.43	0.54
1:P:103:PHE:HE1	1:P:113:HIS:CE1	2.26	0.54
1:P:132:LYS:H	1:P:132:LYS:HD2	1.72	0.54
1:H:245:ARG:HH11	1:H:245:ARG:CG	2.21	0.54
1:H:469:ASP:HB2	1:H:476:ARG:HD2	1.90	0.54
1:J:26:VAL:HG13	1:J:30:HIS:HD2	1.73	0.54
1:P:382:LEU:HA	1:P:385:GLN:HE22	1.72	0.54
1:G:114:VAL:HG21	1:G:137:PHE:HB3	1.88	0.54
1:N:306:LYS:HE3	1:N:329:HIS:HB3	1.89	0.54
1:C:460:PHE:HE1	1:D:130:ILE:HD11	1.73	0.53
1:I:31:LEU:HB3	1:I:35:ILE:HG12	1.90	0.53
1:I:286:ASP:HB3	1:I:341:PHE:HB2	1.89	0.53
1:J:414:LEU:O	1:J:418:MET:HG3	2.08	0.53
1:K:263:LEU:O	1:L:324:SER:HB3	2.07	0.53
1:I:452:CYS:HA	1:I:466:THR:O	2.09	0.53
1:O:441:VAL:HG13	1:O:456:VAL:HB	1.90	0.53
1:R:38:LEU:CD2	1:R:40:ILE:HG12	2.39	0.53
1:R:61:ASP:HB3	1:R:64:VAL:HG13	1.90	0.53
1:C:423:ASN:ND2	2:C:518:HOH:O	2.40	0.53
1:J:76:LYS:HE3	1:J:77:TYR:CE2	2.44	0.53
1:N:138:ARG:NE	1:N:140:VAL:HG12	2.22	0.53
1:P:141:THR:HG23	1:P:145:GLY:HA2	1.89	0.53
1:R:400:GLU:H	1:R:400:GLU:CD	2.14	0.53
1:C:237:SER:HB2	1:R:275:ARG:HB3	1.89	0.53
1:H:61:ASP:HB3	1:H:64:VAL:HG13	1.89	0.53
1:K:286:ASP:HB3	1:K:341:PHE:HB2	1.91	0.53
1:O:15:ARG:HD2	1:O:396:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLU:HG3	1:A:476:ARG:HD3	1.90	0.53
1:D:378:ASN:HB3	1:D:392:ILE:HG12	1.89	0.53
1:F:378:ASN:HB3	1:F:392:ILE:HD11	1.90	0.53
1:C:414:LEU:O	1:C:418:MET:HG3	2.08	0.53
1:D:281:MET:O	1:D:364:GLY:HA3	2.09	0.53
1:N:67:TRP:O	1:N:71:GLU:HG2	2.08	0.53
1:P:378:ASN:OD1	1:P:378:ASN:N	2.41	0.53
1:R:87:HIS:CD2	1:R:158:GLN:HG2	2.44	0.53
1:I:80:CYS:HB2	1:I:186:LEU:HB3	1.91	0.53
1:O:230:PRO:HG2	1:O:247:MET:HE3	1.89	0.53
1:P:96:THR:O	1:P:99:ILE:HG22	2.09	0.53
1:R:327:ASN:O	1:R:328:ILE:HG12	2.08	0.53
1:R:414:LEU:O	1:R:418:MET:HG3	2.08	0.53
1:G:252:PHE:O	1:G:255:PRO:HD2	2.08	0.53
1:F:229:LEU:HD21	1:F:250:TYR:CZ	2.45	0.52
1:N:280:ASN:N	1:N:280:ASN:OD1	2.38	0.52
1:R:74:THR:HG21	1:R:183:GLY:HA3	1.92	0.52
1:K:15:ARG:HG2	1:K:370:TYR:OH	2.08	0.52
1:G:101:ASN:HB2	1:G:105:SER:HB2	1.91	0.52
1:J:303:GLU:CD	1:J:303:GLU:H	2.15	0.52
1:K:242:ILE:HG23	1:K:247:MET:HB2	1.90	0.52
1:K:21:LYS:HE2	1:K:69:ASP:OD1	2.09	0.52
1:N:113:HIS:O	1:N:116:LYS:HG2	2.09	0.52
1:R:308:LEU:O	1:R:312:ILE:HG12	2.10	0.52
1:R:316:SER:HB2	1:R:339:CYS:HB2	1.90	0.52
1:E:140:VAL:HG12	1:E:148:THR:HG23	1.91	0.52
1:J:402:VAL:O	1:J:406:ILE:HG12	2.10	0.52
1:M:151:TRP:CD2	1:M:197:LYS:HD3	2.44	0.52
1:M:229:LEU:HD21	1:M:250:TYR:CZ	2.45	0.52
1:Q:128:ILE:HG22	1:Q:130:ILE:HG12	1.91	0.52
1:Q:130:ILE:HG13	1:Q:323:ARG:HH21	1.74	0.52
1:Q:400:GLU:O	1:Q:404:GLN:HG2	2.09	0.52
1:R:61:ASP:OD1	1:R:62:PRO:HD2	2.10	0.52
1:P:14:ASP:OD1	1:P:14:ASP:N	2.43	0.52
1:Q:349:ASP:CG	1:Q:410:VAL:HB	2.35	0.52
1:A:460:PHE:CE1	1:C:130:ILE:HD11	2.44	0.52
1:C:9:LEU:HB3	1:C:38:LEU:HD12	1.90	0.52
1:L:252:PHE:O	1:L:255:PRO:HD2	2.09	0.52
1:N:34:ALA:HB1	1:N:418:MET:HE2	1.91	0.52
1:R:88:ILE:HG23	1:R:161:LEU:HD21	1.92	0.52
1:A:249:PRO:HD2	1:A:281:MET:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:HH21	1:D:459:ASN:HB3	1.74	0.52
1:B:249:PRO:HG2	1:B:281:MET:HB3	1.90	0.52
1:J:10:ILE:HD11	1:J:367:GLN:HB3	1.90	0.52
1:J:27:VAL:HG22	1:J:31:LEU:HD12	1.92	0.52
1:K:286:ASP:OD1	1:K:286:ASP:N	2.43	0.52
1:A:381:GLU:H	1:A:381:GLU:CD	2.17	0.52
1:C:130:ILE:HD13	1:C:136:PRO:HG3	1.91	0.52
1:G:12:TYR:CB	1:G:15:ARG:HG2	2.39	0.52
1:K:138:ARG:HH11	1:K:159:ILE:HD11	1.73	0.52
1:O:258:LEU:HD12	1:O:285:LEU:HD21	1.91	0.52
1:Q:12:TYR:HB2	1:Q:15:ARG:HG2	1.91	0.52
1:Q:207:GLU:HG2	1:Q:211:TYR:CE2	2.44	0.52
1:R:398:THR:OG1	1:R:400:GLU:HG2	2.10	0.52
1:R:455:PHE:HB3	1:R:464:LYS:CG	2.40	0.52
1:D:130:ILE:HD12	1:D:130:ILE:O	2.10	0.52
1:F:80:CYS:HB2	1:F:186:LEU:HB3	1.91	0.52
1:G:328:ILE:HG13	1:G:329:HIS:CE1	2.45	0.52
1:I:10:ILE:HD12	1:I:39:HIS:CD2	2.46	0.52
1:J:252:PHE:O	1:J:255:PRO:HD2	2.09	0.52
1:P:2:LEU:HD21	1:P:185:ASN:O	2.10	0.52
1:G:9:LEU:HB3	1:G:38:LEU:CD2	2.40	0.51
1:I:245:ARG:O	1:I:246:ASN:HB2	2.10	0.51
1:L:325:ALA:HB1	1:L:333:ALA:CA	2.40	0.51
1:L:431:PHE:HE1	1:L:443:MET:HB3	1.74	0.51
1:M:254:LEU:HD11	1:M:258:LEU:HD22	1.92	0.51
1:R:7:VAL:HG11	1:R:418:MET:HE3	1.92	0.51
1:D:2:LEU:HD12	1:D:3:LEU:HG	1.91	0.51
1:F:469:ASP:OD2	1:F:476:ARG:NH1	2.42	0.51
1:N:53:SER:HB2	1:N:158:GLN:HG3	1.91	0.51
1:O:316:SER:HB2	1:O:339:CYS:HB2	1.93	0.51
1:P:10:ILE:HD11	1:P:367:GLN:OE1	2.10	0.51
1:E:81:VAL:HG22	1:E:184:VAL:HG11	1.93	0.51
1:F:286:ASP:OD1	1:F:286:ASP:N	2.42	0.51
1:G:63:LYS:NZ	2:G:508:HOH:O	2.43	0.51
1:O:130:ILE:HG13	1:O:323:ARG:NH1	2.25	0.51
1:G:316:SER:HB2	1:G:338:THR:O	2.11	0.51
1:K:431:PHE:HB2	1:K:445:TRP:CZ2	2.45	0.51
1:M:287:THR:O	1:M:393:ASN:ND2	2.44	0.51
1:O:27:VAL:HG22	1:O:31:LEU:HD12	1.93	0.51
1:O:130:ILE:HG13	1:O:323:ARG:HH12	1.76	0.51
1:Q:378:ASN:HB3	1:Q:392:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:OG1	1:A:343:ASP:HB2	2.11	0.51
1:B:10:ILE:HD11	1:B:367:GLN:OE1	2.11	0.51
1:B:307:VAL:HG13	1:G:327:ASN:HA	1.93	0.51
1:B:469:ASP:HB3	1:B:472:THR:HG22	1.93	0.51
1:I:228:CYS:HB2	1:I:247:MET:HG2	1.92	0.51
1:N:26:VAL:HA	1:N:29:THR:HG22	1.92	0.51
1:P:67:TRP:CE3	1:P:182:LYS:HE2	2.45	0.51
1:E:479:GLU:O	1:E:480:CYS:C	2.54	0.51
1:N:70:ILE:O	1:N:74:THR:HG23	2.11	0.51
1:P:171:LEU:HD11	1:P:175:TYR:CZ	2.45	0.51
1:C:272:ASN:O	1:C:276:MET:HG2	2.10	0.51
1:L:163:TYR:O	1:L:169:TYR:HE1	1.93	0.51
1:M:139:GLU:HG3	1:M:149:ARG:HG3	1.93	0.51
1:M:151:TRP:CE2	1:M:197:LYS:HD3	2.46	0.51
1:P:382:LEU:HA	1:P:385:GLN:NE2	2.26	0.51
1:E:460:PHE:CE1	1:K:130:ILE:HD11	2.46	0.51
1:H:124:ASP:HA	1:H:127:LYS:HD2	1.92	0.51
1:J:47:ASN:ND2	1:J:89:SER:OG	2.44	0.51
1:N:229:LEU:HD21	1:N:250:TYR:CZ	2.46	0.51
1:Q:286:ASP:OD1	1:Q:356:ARG:NH2	2.41	0.51
1:N:469:ASP:HB2	1:N:476:ARG:HD2	1.93	0.51
1:R:49:ASP:CB	1:R:158:GLN:HE22	2.24	0.51
1:B:127:LYS:NZ	1:C:123:ASP:OD2	2.43	0.50
1:L:144:ASP:OD1	1:L:146:THR:HG22	2.11	0.50
1:Q:381:GLU:O	1:Q:385:GLN:HG3	2.11	0.50
1:B:388:GLU:OE2	1:B:390:ARG:NH1	2.43	0.50
1:E:7:VAL:HG11	1:E:418:MET:HE3	1.93	0.50
1:O:469:ASP:O	1:O:473:GLY:N	2.44	0.50
1:G:142:LEU:HB2	1:G:144:ASP:OD2	2.12	0.50
1:G:323:ARG:NE	2:G:511:HOH:O	2.44	0.50
1:I:242:ILE:HG23	1:I:247:MET:HE3	1.93	0.50
1:N:12:TYR:CD1	1:N:15:ARG:HG2	2.45	0.50
1:O:285:LEU:HD13	1:O:341:PHE:CE2	2.47	0.50
1:A:469:ASP:CB	1:A:476:ARG:HE	2.25	0.50
1:B:273:TRP:CH2	1:B:281:MET:HE1	2.47	0.50
1:E:414:LEU:O	1:E:418:MET:HG3	2.11	0.50
1:I:305:ILE:O	1:I:309:ILE:HG13	2.11	0.50
1:O:289:ASP:HA	1:O:394:ARG:HH21	1.76	0.50
1:O:391:ASP:HA	1:O:394:ARG:HB2	1.92	0.50
1:J:205:LEU:HD11	1:J:232:VAL:HG21	1.93	0.50
1:P:381:GLU:H	1:P:381:GLU:CD	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:131:ARG:O	1:Q:323:ARG:HB3	2.12	0.50
1:R:49:ASP:HB2	1:R:158:GLN:HE22	1.76	0.50
1:P:180:THR:HG21	1:P:224:HIS:HB3	1.94	0.50
1:B:133:GLU:O	1:R:460:PHE:HA	2.12	0.50
1:C:82:ASP:OD1	1:C:188:ARG:HD3	2.11	0.50
1:J:304:LYS:O	1:J:307:VAL:HG22	2.11	0.50
1:J:431:PHE:HE1	1:J:443:MET:HB3	1.77	0.50
1:H:215:ASP:OD1	1:H:245:ARG:HD3	2.12	0.50
1:L:166:ASP:OD1	1:L:170:GLN:NE2	2.44	0.50
1:L:179:LEU:O	1:L:184:VAL:HG13	2.12	0.50
1:M:382:LEU:HG	1:M:391:ASP:HB3	1.92	0.50
1:R:415:LEU:O	1:R:419:LYS:HD2	2.10	0.50
1:C:244:ARG:HA	1:C:279:ARG:HH22	1.76	0.49
1:G:214:LEU:HB3	1:G:247:MET:HE1	1.94	0.49
1:R:61:ASP:O	1:R:64:VAL:HG22	2.11	0.49
1:D:242:ILE:HG23	1:D:247:MET:HB2	1.94	0.49
1:D:335:TYR:CD2	1:D:336:GLN:HG3	2.46	0.49
1:L:82:ASP:OD2	1:L:188:ARG:NH1	2.45	0.49
1:M:469:ASP:O	1:M:473:GLY:N	2.42	0.49
1:B:53:SER:O	1:B:89:SER:HB2	2.12	0.49
1:G:286:ASP:OD1	1:G:286:ASP:N	2.43	0.49
1:I:293:ILE:O	1:I:296:VAL:HG12	2.12	0.49
1:C:469:ASP:O	1:C:473:GLY:N	2.43	0.49
1:J:390:ARG:O	1:J:394:ARG:HG3	2.12	0.49
1:K:188:ARG:NH1	1:K:190:ASP:OD1	2.45	0.49
1:K:209:GLU:CD	1:K:209:GLU:H	2.20	0.49
1:N:404:GLN:HG2	1:N:405:ASP:N	2.26	0.49
1:P:23:LEU:HD23	1:P:73:PHE:CZ	2.48	0.49
1:R:455:PHE:HB3	1:R:464:LYS:HG3	1.94	0.49
1:A:381:GLU:O	1:A:385:GLN:HG2	2.12	0.49
1:B:316:SER:HB2	1:B:338:THR:O	2.11	0.49
1:E:33:GLU:HB2	1:E:419:LYS:HE2	1.94	0.49
1:H:47:ASN:ND2	1:H:89:SER:OG	2.45	0.49
1:M:382:LEU:HD12	1:M:385:GLN:HE22	1.76	0.49
1:N:139:GLU:CD	1:N:147:LYS:HE3	2.36	0.49
1:P:3:LEU:HD11	1:P:186:LEU:HD13	1.93	0.49
1:P:350:ASP:HB3	1:P:461:LYS:O	2.13	0.49
1:P:439:SER:HB3	2:P:509:HOH:O	2.11	0.49
1:P:467:TYR:CE2	1:P:476:ARG:HG3	2.47	0.49
1:Q:243:SER:HB2	1:Q:249:PRO:HG3	1.94	0.49
1:C:469:ASP:HB3	1:C:472:THR:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:LYS:HG2	1:E:178:PHE:CG	2.47	0.49
1:O:288:HIS:HA	1:O:369:TYR:CZ	2.47	0.49
1:P:15:ARG:HG2	1:P:370:TYR:OH	2.12	0.49
1:P:322:ARG:HH12	1:P:334:ILE:C	2.20	0.49
1:Q:374:LEU:HD22	1:Q:405:ASP:HB3	1.95	0.49
1:A:58:LYS:HG2	1:A:178:PHE:CD1	2.48	0.49
1:F:430:HIS:NE2	1:F:432:GLU:OE2	2.41	0.49
1:I:383:MET:HG2	1:I:388:GLU:O	2.13	0.49
1:Q:107:TYR:O	1:Q:110:LEU:HB3	2.13	0.49
1:C:278:PRO:HD2	1:C:281:MET:HE1	1.94	0.49
1:F:258:LEU:HD13	1:F:355:ALA:HB1	1.95	0.49
1:G:253:ALA:O	1:G:256:PRO:HD2	2.13	0.49
1:K:17:GLY:HA3	1:K:22:ASP:HB3	1.93	0.49
1:L:430:HIS:CD2	1:L:446:ARG:HB3	2.48	0.49
1:P:88:ILE:HD11	1:P:111:PHE:CE1	2.48	0.49
1:B:279:ARG:HG3	1:B:280:ASN:N	2.26	0.49
1:K:176:ILE:HG22	1:K:224:HIS:CD2	2.48	0.49
1:N:9:LEU:HD23	1:N:38:LEU:HD11	1.93	0.49
1:P:97:ASP:OD2	1:P:105:SER:OG	2.23	0.49
1:Q:132:LYS:NZ	1:Q:154:PHE:O	2.44	0.49
1:R:171:LEU:HD11	1:R:175:TYR:CE2	2.48	0.49
1:F:80:CYS:HA	1:F:186:LEU:O	2.13	0.49
1:H:112:VAL:HG22	1:H:162:ASN:HB2	1.94	0.49
1:O:8:GLN:HG2	1:O:37:GLY:HA3	1.94	0.49
1:O:132:LYS:HG3	1:O:134:LYS:O	2.13	0.49
1:O:472:THR:O	1:O:474:GLU:HG2	2.13	0.49
1:F:185:ASN:OD1	1:F:185:ASN:N	2.46	0.48
1:G:21:LYS:HE3	1:G:69:ASP:OD1	2.13	0.48
1:K:289:ASP:OD1	1:K:390:ARG:NH1	2.46	0.48
1:L:249:PRO:HD2	1:L:281:MET:HA	1.95	0.48
1:O:419:LYS:HB3	1:O:419:LYS:HE2	1.52	0.48
1:K:460:PHE:HA	1:L:133:GLU:O	2.13	0.48
1:L:432:GLU:HG3	1:L:444:ALA:HB3	1.94	0.48
1:P:139:GLU:OE2	1:P:147:LYS:HB3	2.12	0.48
1:P:382:LEU:HD13	1:P:395:HIS:HA	1.94	0.48
1:R:127:LYS:NZ	2:R:506:HOH:O	2.39	0.48
1:I:247:MET:HE3	1:I:247:MET:HB2	1.68	0.48
1:L:102:GLY:O	1:L:105:SER:HB3	2.14	0.48
1:O:407:GLN:O	1:O:408:LYS:C	2.56	0.48
1:Q:301:PRO:O	1:Q:305:ILE:HG13	2.12	0.48
1:R:85:VAL:O	1:R:161:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:PRO:HD2	1:E:281:MET:HA	1.95	0.48
1:J:33:GLU:HB2	1:J:419:LYS:HG2	1.95	0.48
1:Q:218:ASN:O	1:Q:222:LEU:HG	2.13	0.48
1:D:230:PRO:CG	1:D:247:MET:HE2	2.40	0.48
1:G:272:ASN:O	1:G:276:MET:HG2	2.14	0.48
1:L:33:GLU:HB3	1:L:419:LYS:HD2	1.95	0.48
1:L:244:ARG:HH11	1:L:244:ARG:HG3	1.78	0.48
1:M:142:LEU:HD12	1:M:146:THR:OG1	2.13	0.48
1:B:327:ASN:CB	1:R:307:VAL:HB	2.39	0.48
1:F:383:MET:HE2	1:F:389:LEU:HA	1.96	0.48
1:H:285:LEU:HD13	1:H:341:PHE:CE2	2.49	0.48
1:I:1:MET:HE3	1:I:248:HIS:CE1	2.48	0.48
1:I:103:PHE:HZ	1:I:148:THR:HG21	1.78	0.48
1:C:130:ILE:HG22	1:C:153:THR:HG23	1.94	0.48
1:D:304:LYS:NZ	2:D:504:HOH:O	2.34	0.48
1:E:388:GLU:OE2	1:E:390:ARG:HD3	2.13	0.48
1:F:308:LEU:O	1:F:312:ILE:HG12	2.14	0.48
1:M:383:MET:HE2	1:M:383:MET:HB3	1.79	0.48
1:O:110:LEU:HD11	1:O:161:LEU:HD22	1.96	0.48
1:O:383:MET:HE2	1:O:389:LEU:HA	1.96	0.48
1:R:287:THR:O	1:R:393:ASN:ND2	2.47	0.48
1:E:265:ALA:HB3	1:K:324:SER:HB2	1.95	0.48
1:K:135:GLU:HG2	1:K:136:PRO:HD2	1.94	0.48
1:N:9:LEU:HB3	1:N:38:LEU:HD12	1.95	0.48
1:O:24:TYR:HA	1:O:73:PHE:CZ	2.49	0.48
1:D:138:ARG:HD3	1:D:140:VAL:HG12	1.96	0.48
1:K:8:GLN:HG2	1:K:37:GLY:HA3	1.96	0.48
1:R:8:GLN:HA	1:R:37:GLY:O	2.13	0.48
1:R:474:GLU:O	1:R:474:GLU:HG3	2.13	0.48
1:C:469:ASP:CB	1:C:472:THR:HG22	2.44	0.48
1:C:472:THR:HG23	1:C:474:GLU:HB3	1.96	0.48
1:E:76:LYS:NZ	1:N:216:TRP:HE1	2.12	0.48
1:F:249:PRO:HD2	1:F:280:ASN:O	2.14	0.47
1:I:152:CYS:HB2	1:I:158:GLN:O	2.14	0.47
1:J:98:PHE:O	1:J:102:GLY:HA2	2.13	0.47
1:J:286:ASP:OD2	1:J:369:TYR:HB3	2.14	0.47
1:P:252:PHE:O	1:P:255:PRO:HD2	2.14	0.47
1:R:113:HIS:O	1:R:116:LYS:HG2	2.14	0.47
1:B:272:ASN:O	1:B:276:MET:HG2	2.14	0.47
1:F:254:LEU:HD13	1:F:273:TRP:CZ3	2.49	0.47
1:H:388:GLU:HG3	1:H:391:ASP:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:47:ASN:OD1	1:O:47:ASN:N	2.47	0.47
1:Q:15:ARG:NH1	1:Q:394:ARG:O	2.47	0.47
1:D:85:VAL:HA	1:D:172:MET:HE3	1.95	0.47
1:B:450:TYR:CE1	1:B:470:VAL:HG12	2.50	0.47
1:F:42:PRO:O	2:F:501:HOH:O	2.20	0.47
1:F:324:SER:OG	2:F:502:HOH:O	2.20	0.47
1:G:82:ASP:OD1	1:G:188:ARG:HD3	2.14	0.47
1:I:154:PHE:O	1:I:158:GLN:HB2	2.15	0.47
1:N:315:ARG:NH1	1:N:346:MET:HE2	2.30	0.47
1:P:182:LYS:HD2	1:P:182:LYS:N	2.28	0.47
1:A:81:VAL:HG22	1:A:184:VAL:HG11	1.96	0.47
1:H:38:LEU:HD22	1:H:40:ILE:CG1	2.44	0.47
1:H:252:PHE:O	1:H:255:PRO:HD2	2.14	0.47
1:I:12:TYR:CE2	1:I:394:ARG:HG2	2.49	0.47
1:I:241:ALA:O	1:I:245:ARG:HD2	2.14	0.47
1:M:218:ASN:HB2	1:M:247:MET:HE3	1.96	0.47
1:P:138:ARG:O	1:P:138:ARG:HG3	2.14	0.47
1:P:356:ARG:HG3	1:P:414:LEU:HD13	1.96	0.47
1:R:66:THR:HG22	1:R:69:ASP:CG	2.39	0.47
1:A:469:ASP:HB2	1:A:476:ARG:HE	1.80	0.47
1:H:306:LYS:HE3	1:H:306:LYS:HB2	1.64	0.47
1:R:46:SER:CB	1:R:51:GLY:HA2	2.43	0.47
1:R:272:ASN:O	1:R:276:MET:HG2	2.15	0.47
1:H:110:LEU:HD11	1:H:161:LEU:HD22	1.97	0.47
1:I:12:TYR:HE2	1:I:394:ARG:HG2	1.80	0.47
1:K:151:TRP:CD2	1:K:197:LYS:HD3	2.50	0.47
1:L:286:ASP:OD2	1:L:286:ASP:N	2.45	0.47
1:M:57:HIS:CE1	1:M:84:THR:H	2.33	0.47
1:M:88:ILE:HG12	1:M:161:LEU:HD21	1.97	0.47
1:N:257:LEU:HD21	1:N:270:LEU:HA	1.97	0.47
1:N:404:GLN:HE21	1:N:404:GLN:HB3	1.49	0.47
1:P:123:ASP:O	1:P:127:LYS:HG3	2.14	0.47
1:Q:80:CYS:HA	1:Q:186:LEU:O	2.15	0.47
1:Q:88:ILE:HG12	1:Q:161:LEU:HD21	1.96	0.47
1:Q:242:ILE:O	1:Q:245:ARG:HB2	2.15	0.47
1:R:12:TYR:HB2	1:R:15:ARG:CG	2.43	0.47
1:R:92:SER:O	1:R:96:THR:HG23	2.14	0.47
1:R:240:TYR:O	1:R:244:ARG:HD3	2.14	0.47
1:B:2:LEU:HD12	1:B:2:LEU:HA	1.67	0.47
1:H:382:LEU:HG	1:H:391:ASP:HB3	1.97	0.47
1:I:239:GLN:NE2	1:I:250:TYR:H	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:274:LEU:HD13	1:M:443:MET:HE3	1.96	0.47
1:R:235:HIS:HD2	1:R:297:GLU:OE1	1.98	0.47
1:A:53:SER:O	1:A:89:SER:HB2	2.15	0.47
1:G:47:ASN:ND2	1:G:89:SER:OG	2.34	0.47
1:G:466:THR:HG23	1:G:475:THR:HG23	1.96	0.47
1:J:457:ASP:HB3	1:J:462:THR:CG2	2.45	0.47
1:P:41:LEU:HD21	1:P:288:HIS:CG	2.50	0.47
1:E:138:ARG:HH11	1:E:159:ILE:HD11	1.80	0.47
1:E:466:THR:HG22	1:E:477:HIS:CD2	2.50	0.47
1:G:244:ARG:HG3	1:G:244:ARG:HH11	1.80	0.47
1:J:472:THR:HG21	1:J:476:ARG:HH22	1.80	0.47
1:K:330:SER:O	1:K:334:ILE:HD12	2.14	0.47
1:K:400:GLU:H	1:K:400:GLU:CD	2.23	0.47
1:L:58:LYS:HG2	1:L:178:PHE:CG	2.50	0.47
1:L:62:PRO:HG2	1:R:63:LYS:HG2	1.97	0.47
1:L:79:LEU:HD23	1:L:184:VAL:HG12	1.97	0.47
1:A:400:GLU:HG3	1:A:404:GLN:NE2	2.28	0.46
1:E:91:GLU:OE2	2:E:502:HOH:O	2.21	0.46
1:G:404:GLN:NE2	1:L:404:GLN:O	2.42	0.46
1:H:132:LYS:HD3	1:H:153:THR:O	2.15	0.46
1:H:192:PHE:CE1	1:H:214:LEU:HD11	2.50	0.46
1:J:472:THR:HG21	1:J:476:ARG:NH2	2.30	0.46
1:P:59:GLU:HA	1:P:67:TRP:HE1	1.80	0.46
1:R:12:TYR:CD2	1:R:15:ARG:HG2	2.50	0.46
1:R:207:GLU:HG2	1:R:211:TYR:CE2	2.49	0.46
1:B:80:CYS:HA	1:B:186:LEU:O	2.15	0.46
1:L:236:THR:N	2:L:507:HOH:O	2.44	0.46
1:O:87:HIS:CD2	1:O:158:GLN:HG2	2.50	0.46
1:O:240:TYR:O	1:O:244:ARG:HG2	2.15	0.46
1:O:286:ASP:HB3	1:O:341:PHE:HB2	1.97	0.46
1:C:79:LEU:HD23	1:C:184:VAL:HG22	1.96	0.46
1:D:14:ASP:OD1	1:D:14:ASP:N	2.47	0.46
1:D:385:GLN:H	1:D:385:GLN:HG3	1.57	0.46
1:H:303:GLU:HG3	1:H:304:LYS:N	2.30	0.46
1:J:306:LYS:HG3	1:J:331:VAL:HG23	1.98	0.46
1:M:215:ASP:O	1:M:219:GLN:HG2	2.15	0.46
1:N:222:LEU:HD12	1:N:226:ALA:O	2.16	0.46
1:A:474:GLU:CG	1:A:476:ARG:HD3	2.44	0.46
1:D:249:PRO:HD2	1:D:281:MET:HA	1.98	0.46
1:G:236:THR:HG22	2:G:574:HOH:O	2.14	0.46
1:K:88:ILE:HG12	1:K:161:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:464:LYS:HB2	1:R:464:LYS:HE3	1.54	0.46
1:F:33:GLU:HB2	1:F:419:LYS:HD3	1.98	0.46
1:P:2:LEU:HD23	1:P:227:GLU:HB2	1.98	0.46
1:R:29:THR:HB	1:R:30:HIS:ND1	2.30	0.46
1:A:237:SER:HB3	1:B:276:MET:SD	2.55	0.46
1:B:205:LEU:HD21	1:B:232:VAL:HG11	1.96	0.46
1:E:241:ALA:O	1:E:245:ARG:HG3	2.16	0.46
1:H:196:THR:OG1	2:H:501:HOH:O	2.21	0.46
1:J:31:LEU:HD13	1:J:35:ILE:HD13	1.97	0.46
1:K:9:LEU:HD23	1:K:38:LEU:HD11	1.97	0.46
1:L:277:CYS:HB2	1:L:281:MET:HE1	1.97	0.46
1:M:466:THR:HG22	1:M:477:HIS:ND1	2.30	0.46
1:N:241:ALA:O	1:N:245:ARG:HD2	2.15	0.46
1:O:3:LEU:HD11	1:O:186:LEU:HD13	1.96	0.46
1:Q:12:TYR:CB	1:Q:15:ARG:HG2	2.45	0.46
1:E:69:ASP:OD1	2:E:503:HOH:O	2.21	0.46
1:G:472:THR:HG22	1:G:474:GLU:HB3	1.97	0.46
1:I:125:MET:HE1	1:I:137:PHE:CZ	2.51	0.46
1:J:2:LEU:HG	1:J:227:GLU:OE2	2.15	0.46
1:N:58:LYS:HE3	1:N:174:SER:OG	2.16	0.46
1:O:402:VAL:O	1:O:406:ILE:HG12	2.16	0.46
1:Q:179:LEU:O	1:Q:184:VAL:HG13	2.15	0.46
1:R:4:LYS:HD2	1:R:78:ASP:CG	2.40	0.46
1:E:80:CYS:HB2	1:E:186:LEU:HB3	1.97	0.46
1:I:321:MET:HE3	1:I:321:MET:HB3	1.70	0.46
1:N:389:LEU:O	1:N:392:ILE:HG23	2.15	0.46
1:Q:269:TYR:N	2:Q:509:HOH:O	2.48	0.46
1:R:13:PRO:HG2	1:R:43:PHE:HB3	1.97	0.46
1:A:66:THR:HG22	1:A:69:ASP:CG	2.40	0.46
1:B:400:GLU:CD	1:B:400:GLU:H	2.24	0.46
1:D:327:ASN:O	1:D:330:SER:HB3	2.16	0.46
1:E:10:ILE:HD11	1:E:367:GLN:HB3	1.98	0.46
1:L:10:ILE:HD11	1:L:367:GLN:HB3	1.97	0.46
1:M:277:CYS:HB2	1:M:281:MET:HE1	1.97	0.46
1:Q:231:GLU:O	1:Q:231:GLU:HG3	2.15	0.46
1:R:7:VAL:HG12	1:R:35:ILE:HG22	1.98	0.46
1:F:381:GLU:H	1:F:381:GLU:CD	2.23	0.46
1:H:130:ILE:HG22	1:H:153:THR:HG23	1.98	0.46
1:I:239:GLN:HG3	1:I:249:PRO:CB	2.42	0.46
1:O:213:ILE:O	1:O:217:VAL:HG23	2.16	0.46
1:O:453:HIS:HD2	2:O:530:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:382:LEU:HA	1:Q:385:GLN:CD	2.41	0.46
1:R:39:HIS:HB2	1:R:80:CYS:HB3	1.98	0.46
1:B:12:TYR:HB2	1:B:15:ARG:HG2	1.98	0.45
1:C:270:LEU:HD23	1:C:441:VAL:HG21	1.97	0.45
1:D:123:ASP:O	1:D:127:LYS:HG3	2.16	0.45
1:F:142:LEU:HD12	1:F:146:THR:HB	1.98	0.45
1:F:328:ILE:HG12	1:O:311:ASN:HA	1.97	0.45
1:H:382:LEU:O	1:H:385:GLN:HG3	2.16	0.45
1:I:120:ILE:HG21	1:I:125:MET:HE2	1.97	0.45
1:I:406:ILE:HA	1:I:411:VAL:HG11	1.97	0.45
1:L:399:LEU:O	1:L:403:GLU:HG2	2.15	0.45
1:L:439:SER:OG	1:L:459:ASN:OD1	2.32	0.45
1:M:45:PRO:HA	2:M:507:HOH:O	2.16	0.45
1:M:192:PHE:CE1	1:M:214:LEU:HD11	2.51	0.45
1:N:130:ILE:HD13	1:N:136:PRO:HG3	1.98	0.45
1:O:82:ASP:HB3	1:O:190:ASP:OD2	2.16	0.45
1:O:215:ASP:O	1:O:219:GLN:HG3	2.16	0.45
1:P:255:PRO:HB2	1:P:256:PRO:HD3	1.97	0.45
1:P:383:MET:HE3	1:P:383:MET:HB3	1.75	0.45
1:Q:160:ASP:OD2	1:Q:197:LYS:NZ	2.47	0.45
1:G:285:LEU:HD13	1:G:341:PHE:CE2	2.51	0.45
1:H:286:ASP:HB3	1:H:341:PHE:HB2	1.98	0.45
1:I:140:VAL:HG22	1:I:148:THR:O	2.16	0.45
1:L:16:ILE:HG23	1:L:402:VAL:HG21	1.96	0.45
1:N:400:GLU:CD	1:N:400:GLU:H	2.24	0.45
1:A:454:LEU:HD11	1:A:456:VAL:HG23	1.98	0.45
1:H:47:ASN:ND2	1:H:91:GLU:HG3	2.26	0.45
1:J:243:SER:OG	1:J:279:ARG:HG3	2.15	0.45
1:K:202:SER:O	1:K:203:CYS:HB2	2.15	0.45
1:N:9:LEU:HB3	1:N:38:LEU:CD1	2.46	0.45
1:P:441:VAL:HG13	1:P:456:VAL:HB	1.98	0.45
1:Q:325:ALA:HB1	1:Q:333:ALA:HB1	1.98	0.45
1:Q:331:VAL:HG23	1:Q:332:GLY:N	2.32	0.45
1:A:38:LEU:CD2	1:A:40:ILE:CG1	2.94	0.45
1:A:88:ILE:HG12	1:A:161:LEU:HD21	1.99	0.45
1:F:130:ILE:HD11	1:O:460:PHE:HE1	1.82	0.45
1:H:272:ASN:O	1:H:276:MET:HG2	2.17	0.45
1:J:382:LEU:O	1:J:385:GLN:HG2	2.17	0.45
1:K:321:MET:HB3	1:K:321:MET:HE3	1.80	0.45
1:K:391:ASP:HA	1:K:394:ARG:HB2	1.97	0.45
1:L:12:TYR:CB	1:L:15:ARG:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:LEU:HD23	1:L:38:LEU:HA	1.78	0.45
1:L:382:LEU:HG	1:L:391:ASP:HB3	1.98	0.45
1:R:406:ILE:HD12	1:R:415:LEU:HD11	1.99	0.45
1:M:252:PHE:O	1:M:255:PRO:HD2	2.17	0.45
1:N:79:LEU:HD23	1:N:184:VAL:HG22	1.98	0.45
1:P:285:LEU:HD13	1:P:341:PHE:CE2	2.51	0.45
1:Q:112:VAL:HG22	1:Q:162:ASN:HB2	1.98	0.45
1:R:12:TYR:HB2	1:R:15:ARG:CB	2.44	0.45
1:R:19:ASN:OD1	1:R:21:LYS:HB2	2.16	0.45
1:C:293:ILE:O	1:C:296:VAL:HG12	2.17	0.45
1:J:177:GLY:HA2	1:J:224:HIS:CD2	2.52	0.45
1:K:169:TYR:HB3	1:K:216:TRP:CZ2	2.51	0.45
1:D:257:LEU:HD21	1:D:270:LEU:HA	1.99	0.45
1:H:467:TYR:CE2	1:H:476:ARG:HD3	2.51	0.45
1:I:81:VAL:HG22	1:I:184:VAL:HG11	1.99	0.45
1:K:453:HIS:HB3	1:K:466:THR:OG1	2.16	0.45
1:L:12:TYR:O	2:L:501:HOH:O	2.21	0.45
1:P:285:LEU:HB2	1:P:356:ARG:NH1	2.32	0.45
1:D:385:GLN:HE21	1:D:385:GLN:HB2	1.47	0.45
1:F:252:PHE:O	1:F:255:PRO:HD2	2.17	0.45
1:G:100:ALA:HA	1:G:143:SER:OG	2.17	0.45
1:J:95:PHE:CE2	1:J:99:ILE:HD11	2.51	0.45
1:K:128:ILE:HA	1:K:202:SER:O	2.17	0.45
1:N:15:ARG:HG3	1:N:370:TYR:OH	2.16	0.45
1:O:218:ASN:ND2	1:O:247:MET:HG3	2.31	0.45
1:O:345:LEU:HD23	1:O:345:LEU:HA	1.86	0.45
1:Q:53:SER:O	1:Q:89:SER:HB2	2.17	0.45
1:Q:130:ILE:CD1	1:Q:136:PRO:HG3	2.44	0.45
1:Q:322:ARG:NH1	1:Q:334:ILE:O	2.50	0.45
1:D:120:ILE:HG22	1:D:125:MET:HG2	1.99	0.45
1:G:192:PHE:HE1	1:G:232:VAL:HG22	1.81	0.45
1:L:308:LEU:HD12	1:L:312:ILE:HD13	1.99	0.45
1:M:388:GLU:HG3	1:M:391:ASP:H	1.82	0.45
1:M:469:ASP:HB3	1:M:472:THR:HB	1.97	0.45
1:B:323:ARG:NH2	2:B:505:HOH:O	2.42	0.45
1:C:460:PHE:CE1	1:D:130:ILE:HD11	2.51	0.45
1:H:12:TYR:CD1	1:H:15:ARG:HG2	2.52	0.45
1:H:125:MET:HE3	1:H:125:MET:HB3	1.82	0.45
1:L:380:HIS:CD2	1:L:392:ILE:HD11	2.52	0.45
1:N:110:LEU:HD23	1:N:111:PHE:CZ	2.52	0.45
1:N:135:GLU:HB3	1:N:137:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:389:LEU:O	1:O:392:ILE:HG22	2.17	0.45
1:D:237:SER:HB2	1:G:275:ARG:HB3	1.98	0.44
1:I:252:PHE:O	1:I:255:PRO:HD2	2.16	0.44
1:K:38:LEU:HD13	1:K:38:LEU:HA	1.83	0.44
1:L:70:ILE:O	1:L:74:THR:HG23	2.17	0.44
1:M:16:ILE:HG23	1:M:402:VAL:HG21	1.99	0.44
1:M:94:GLU:OE1	1:M:94:GLU:N	2.43	0.44
1:O:151:TRP:N	2:O:511:HOH:O	2.50	0.44
1:A:177:GLY:HA2	1:A:224:HIS:CD2	2.51	0.44
1:B:123:ASP:OD1	2:B:501:HOH:O	2.21	0.44
1:N:57:HIS:HB2	1:N:175:TYR:CD1	2.52	0.44
1:P:41:LEU:HB3	1:P:42:PRO:HD2	1.99	0.44
1:A:244:ARG:NH1	1:A:244:ARG:HG3	2.33	0.44
1:B:12:TYR:CD2	1:B:15:ARG:HG2	2.52	0.44
1:C:476:ARG:CZ	1:C:476:ARG:HB3	2.48	0.44
1:I:346:MET:HB2	1:I:346:MET:HE3	1.69	0.44
1:J:192:PHE:CE1	1:J:214:LEU:HD11	2.52	0.44
1:K:33:GLU:CB	1:K:419:LYS:HG2	2.43	0.44
1:M:286:ASP:CG	1:M:369:TYR:HB3	2.42	0.44
1:O:452:CYS:HA	1:O:466:THR:O	2.18	0.44
1:P:469:ASP:O	1:P:473:GLY:N	2.40	0.44
1:Q:385:GLN:HG3	1:Q:385:GLN:H	1.58	0.44
1:R:101:ASN:HB2	1:R:105:SER:HB2	1.99	0.44
1:A:185:ASN:OD1	1:A:185:ASN:N	2.48	0.44
1:E:265:ALA:HB2	1:K:324:SER:HB2	1.99	0.44
1:M:286:ASP:HB3	1:M:341:PHE:HB2	1.99	0.44
1:Q:449:ASP:HB3	1:Q:470:VAL:HG12	1.98	0.44
1:J:15:ARG:HG2	1:J:370:TYR:OH	2.18	0.44
1:M:20:LEU:HD12	1:M:64:VAL:HG23	1.99	0.44
1:M:76:LYS:HE2	1:M:76:LYS:HB3	1.73	0.44
1:O:244:ARG:HA	1:O:244:ARG:HD3	1.91	0.44
1:P:19:ASN:O	1:P:22:ASP:HB2	2.18	0.44
1:P:425:PRO:HG2	1:P:450:TYR:CE1	2.53	0.44
1:R:68:ASP:HA	1:R:71:GLU:HG3	1.99	0.44
1:A:244:ARG:HG3	1:A:244:ARG:HH11	1.81	0.44
1:H:152:CYS:HB2	1:H:158:GLN:O	2.18	0.44
1:H:205:LEU:HD11	1:H:232:VAL:HG21	1.99	0.44
1:I:10:ILE:HD12	1:I:39:HIS:HD2	1.82	0.44
1:L:12:TYR:CG	1:L:15:ARG:HG2	2.53	0.44
1:L:15:ARG:HG3	1:L:370:TYR:OH	2.17	0.44
1:P:406:ILE:HA	1:P:411:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:SER:O	1:E:89:SER:HB2	2.17	0.44
1:F:1:MET:HG2	1:F:3:LEU:O	2.18	0.44
1:P:144:ASP:OD2	1:P:146:THR:HB	2.18	0.44
1:R:156:GLU:H	1:R:156:GLU:HG2	1.58	0.44
1:R:381:GLU:H	1:R:381:GLU:HG2	1.43	0.44
1:R:391:ASP:HA	1:R:394:ARG:HG3	1.98	0.44
1:F:382:LEU:HG	1:F:391:ASP:HB3	2.00	0.44
1:G:81:VAL:HG21	1:G:179:LEU:HD22	1.99	0.44
1:G:315:ARG:HD2	1:G:343:ASP:O	2.18	0.44
1:L:219:GLN:HG3	1:L:220:VAL:N	2.32	0.44
1:N:29:THR:HG23	1:N:30:HIS:CG	2.52	0.44
1:R:450:TYR:CE2	1:R:470:VAL:HG22	2.53	0.44
1:D:67:TRP:CE3	1:D:182:LYS:HG3	2.53	0.44
1:D:272:ASN:O	1:D:276:MET:HG2	2.18	0.44
1:I:252:PHE:O	2:I:501:HOH:O	2.21	0.44
1:P:381:GLU:HA	1:P:384:GLU:HG2	2.00	0.44
1:Q:191:ALA:HB1	1:Q:194:TYR:HD2	1.83	0.44
1:R:8:GLN:HG2	1:R:37:GLY:HA3	2.00	0.44
1:D:207:GLU:HG2	1:D:211:TYR:CE2	2.53	0.43
1:E:88:ILE:HG12	1:E:161:LEU:HD21	1.99	0.43
1:E:285:LEU:HD13	1:E:341:PHE:CE2	2.53	0.43
1:F:53:SER:O	1:F:89:SER:HB2	2.17	0.43
1:K:61:ASP:O	1:K:64:VAL:HG22	2.17	0.43
1:O:109:ASP:HB2	1:O:167:LEU:HD12	1.99	0.43
1:Q:317:ALA:O	1:Q:318:ASP:C	2.60	0.43
1:R:53:SER:HB2	1:R:158:GLN:NE2	2.33	0.43
1:C:177:GLY:HA2	1:C:224:HIS:CD2	2.53	0.43
1:D:144:ASP:OD1	1:D:146:THR:OG1	2.30	0.43
1:J:179:LEU:O	1:J:184:VAL:HG13	2.18	0.43
1:O:82:ASP:OD2	1:O:188:ARG:HD3	2.18	0.43
1:O:116:LYS:HE2	1:O:117:PHE:CE2	2.52	0.43
1:O:322:ARG:HG2	1:O:335:TYR:HB2	2.00	0.43
1:P:147:LYS:HB2	1:P:147:LYS:HE3	1.39	0.43
1:Q:74:THR:HG21	1:Q:182:LYS:O	2.19	0.43
1:B:254:LEU:HD11	1:B:258:LEU:HD22	1.99	0.43
1:C:399:LEU:HA	1:C:399:LEU:HD23	1.75	0.43
1:E:459:ASN:HB3	1:K:323:ARG:NH1	2.33	0.43
1:H:188:ARG:NH1	1:H:190:ASP:OD1	2.47	0.43
1:L:293:ILE:O	1:L:296:VAL:HG12	2.19	0.43
1:L:303:GLU:HA	1:L:303:GLU:OE1	2.18	0.43
1:O:29:THR:HG23	1:O:30:HIS:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:34:ALA:HB1	1:P:418:MET:HE2	1.99	0.43
1:P:141:THR:CG2	1:P:145:GLY:HA2	2.48	0.43
1:P:292:CYS:SG	1:P:294:PRO:HD2	2.58	0.43
1:P:303:GLU:HG2	2:P:535:HOH:O	2.18	0.43
1:Q:380:HIS:O	1:Q:384:GLU:HG2	2.17	0.43
1:R:315:ARG:HD3	1:R:346:MET:HG2	2.00	0.43
1:B:207:GLU:HG2	1:B:211:TYR:CE2	2.54	0.43
1:C:409:PRO:O	1:C:413:ARG:HG3	2.17	0.43
1:K:79:LEU:CD2	1:K:184:VAL:HG12	2.48	0.43
1:K:127:LYS:HE2	1:K:127:LYS:HB2	1.51	0.43
1:P:7:VAL:HG11	1:P:418:MET:HE3	2.00	0.43
1:P:308:LEU:O	1:P:312:ILE:HG12	2.17	0.43
1:Q:241:ALA:O	1:Q:245:ARG:HG2	2.18	0.43
1:R:79:LEU:HD13	1:R:81:VAL:HG13	1.99	0.43
1:D:321:MET:HE2	1:D:321:MET:HB3	1.83	0.43
1:G:287:THR:O	1:G:393:ASN:ND2	2.51	0.43
1:L:130:ILE:HG22	1:L:153:THR:HG23	2.00	0.43
1:L:277:CYS:O	1:L:279:ARG:NH2	2.52	0.43
1:M:70:ILE:O	1:M:74:THR:HG23	2.18	0.43
1:R:153:THR:HG23	1:R:154:PHE:CD1	2.54	0.43
1:A:309:ILE:HD13	1:A:334:ILE:HG13	2.01	0.43
1:B:81:VAL:HG22	1:B:184:VAL:HG11	2.00	0.43
1:F:88:ILE:HG12	1:F:161:LEU:HD21	2.00	0.43
1:G:323:ARG:NH2	2:G:511:HOH:O	2.51	0.43
1:M:57:HIS:HE1	1:M:84:THR:H	1.66	0.43
1:O:97:ASP:HB3	1:O:107:TYR:HD2	1.84	0.43
1:O:400:GLU:CD	1:O:400:GLU:H	2.26	0.43
1:P:240:TYR:CE1	1:P:278:PRO:HG3	2.53	0.43
1:Q:407:GLN:O	1:Q:408:LYS:C	2.61	0.43
1:R:450:TYR:HE2	1:R:470:VAL:HG13	1.84	0.43
1:A:16:ILE:HG23	1:A:402:VAL:HG21	2.00	0.43
1:D:63:LYS:HB3	1:D:63:LYS:HE3	1.84	0.43
1:E:132:LYS:HG2	2:E:508:HOH:O	2.18	0.43
1:G:245:ARG:HB3	1:G:247:MET:HE3	2.01	0.43
1:H:74:THR:HG21	1:H:182:LYS:O	2.18	0.43
1:J:31:LEU:O	1:J:32:SER:C	2.59	0.43
1:K:258:LEU:HD21	1:K:358:ILE:HG21	2.00	0.43
1:K:449:ASP:OD1	1:K:449:ASP:N	2.50	0.43
1:B:109:ASP:OD2	1:B:165:SER:HB2	2.19	0.43
1:B:213:ILE:O	1:B:217:VAL:HG23	2.18	0.43
1:E:322:ARG:HD3	1:E:335:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:43:PHE:HE2	1:K:67:TRP:CH2	2.36	0.43
1:K:179:LEU:O	1:K:184:VAL:HG13	2.19	0.43
1:K:292:CYS:SG	1:K:294:PRO:HD2	2.58	0.43
1:M:417:LEU:HD23	1:M:417:LEU:HA	1.85	0.43
1:Q:254:LEU:HD13	1:Q:273:TRP:CZ3	2.54	0.43
1:Q:293:ILE:HD11	1:Q:337:LEU:HD11	2.00	0.43
1:A:413:ARG:NE	1:A:480:CYS:OXT	2.32	0.43
1:D:240:TYR:O	1:D:244:ARG:HD3	2.18	0.43
1:F:312:ILE:HD13	1:F:315:ARG:NH2	2.34	0.43
1:G:361:PHE:HB3	1:G:443:MET:HE2	2.01	0.43
1:L:257:LEU:HD21	1:L:270:LEU:HA	2.00	0.43
1:M:144:ASP:CG	1:M:146:THR:HG1	2.18	0.43
1:O:76:LYS:HD3	1:O:77:TYR:CZ	2.53	0.43
1:O:321:MET:HE3	1:O:321:MET:HB3	1.67	0.43
1:P:116:LYS:HE3	1:P:117:PHE:CZ	2.53	0.43
1:P:249:PRO:HD3	1:P:280:ASN:HD22	1.83	0.43
1:R:2:LEU:HD12	1:R:3:LEU:HG	2.01	0.43
1:R:44:PHE:HB2	1:R:54:PRO:HB3	2.01	0.43
1:R:478:LEU:HD12	1:R:479:GLU:N	2.33	0.43
1:A:95:PHE:CE2	1:A:99:ILE:HD11	2.53	0.43
1:A:469:ASP:O	1:A:473:GLY:N	2.44	0.43
1:C:152:CYS:HA	1:C:160:ASP:OD1	2.19	0.43
1:D:125:MET:HA	1:D:128:ILE:HD12	2.01	0.43
1:D:327:ASN:ND2	1:D:330:SER:HB2	2.34	0.43
1:F:135:GLU:HG2	1:O:460:PHE:CD1	2.53	0.43
1:I:306:LYS:HE2	1:I:310:ASP:OD1	2.19	0.43
1:I:424:TYR:HA	1:I:425:PRO:HD3	1.91	0.43
1:M:209:GLU:OE1	1:M:209:GLU:N	2.51	0.43
1:N:439:SER:O	1:N:458:LEU:HB2	2.17	0.43
1:O:218:ASN:O	1:O:222:LEU:HG	2.19	0.43
1:C:395:HIS:NE2	1:C:396:TYR:O	2.52	0.42
1:I:70:ILE:HD13	1:I:70:ILE:HA	1.87	0.42
1:L:61:ASP:OD1	1:L:64:VAL:HG13	2.19	0.42
1:L:321:MET:HE3	1:L:321:MET:HB2	1.89	0.42
1:O:23:LEU:HG	1:O:73:PHE:HZ	1.83	0.42
1:R:66:THR:HG23	1:R:68:ASP:H	1.83	0.42
1:B:382:LEU:HG	1:B:391:ASP:HB3	2.00	0.42
1:D:235:HIS:ND1	1:D:237:SER:OG	2.38	0.42
1:D:346:MET:HE3	1:D:346:MET:HB2	1.87	0.42
1:G:425:PRO:HG2	1:G:450:TYR:CE2	2.54	0.42
1:I:381:GLU:O	1:I:385:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:154:PHE:HB2	1:N:155:THR:H	1.63	0.42
1:N:408:LYS:HB2	1:N:408:LYS:HE3	1.74	0.42
1:B:316:SER:HB3	1:B:339:CYS:HB3	2.01	0.42
1:B:429:GLY:HA3	1:B:446:ARG:O	2.19	0.42
1:D:12:TYR:N	2:D:510:HOH:O	2.44	0.42
1:D:252:PHE:O	1:D:255:PRO:HD2	2.19	0.42
1:D:284:VAL:O	1:D:285:LEU:HD23	2.20	0.42
1:G:446:ARG:HB2	1:G:451:TYR:HD1	1.84	0.42
1:L:31:LEU:HB3	1:L:35:ILE:HG12	2.02	0.42
1:L:267:SER:O	1:L:271:LYS:HG3	2.20	0.42
1:R:265:ALA:HA	1:R:458:LEU:HB3	1.99	0.42
1:R:456:VAL:HG22	1:R:463:VAL:HG22	2.01	0.42
1:C:350:ASP:HB3	1:C:461:LYS:O	2.19	0.42
1:C:459:ASN:ND2	2:C:528:HOH:O	2.51	0.42
1:G:360:PHE:HD1	1:G:417:LEU:HD22	1.84	0.42
1:J:71:GLU:HA	1:J:74:THR:OG1	2.20	0.42
1:K:110:LEU:HD23	1:K:111:PHE:CZ	2.55	0.42
1:N:286:ASP:HB3	1:N:341:PHE:HB2	2.02	0.42
1:O:20:LEU:HD12	1:O:65:GLY:HA3	2.00	0.42
1:P:382:LEU:O	1:P:386:SER:HB3	2.19	0.42
1:R:421:ARG:HA	1:R:427:PHE:CE2	2.54	0.42
1:B:12:TYR:HB2	1:B:15:ARG:HB2	2.01	0.42
1:B:292:CYS:SG	1:B:294:PRO:HD2	2.58	0.42
1:B:474:GLU:H	1:B:474:GLU:HG2	1.69	0.42
1:D:130:ILE:HG22	1:D:153:THR:HG23	2.00	0.42
1:D:379:ASP:OD2	1:D:395:HIS:HD2	2.02	0.42
1:E:432:GLU:HG3	1:E:444:ALA:HB3	2.01	0.42
1:F:100:ALA:HA	1:F:143:SER:HB3	2.01	0.42
1:G:15:ARG:HD3	1:G:396:TYR:CE2	2.54	0.42
1:G:378:ASN:HB3	1:G:392:ILE:HG12	2.01	0.42
1:L:458:LEU:O	1:L:461:LYS:NZ	2.34	0.42
1:O:70:ILE:H	1:O:70:ILE:HG12	1.39	0.42
1:P:142:LEU:HD12	1:P:146:THR:HG22	2.02	0.42
1:P:381:GLU:O	1:P:384:GLU:HB2	2.20	0.42
1:Q:309:ILE:HG21	1:Q:334:ILE:HD12	2.01	0.42
1:R:47:ASN:ND2	1:R:90:ASP:OD1	2.52	0.42
1:R:207:GLU:HG2	1:R:211:TYR:HE2	1.83	0.42
1:E:424:TYR:HA	1:E:425:PRO:HD3	1.92	0.42
1:H:247:MET:HE3	1:H:247:MET:HB2	1.90	0.42
1:I:309:ILE:HG23	1:I:337:LEU:HD21	2.01	0.42
1:L:76:LYS:HE2	1:L:76:LYS:HB3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:325:ALA:CB	1:L:333:ALA:HA	2.48	0.42
1:L:386:SER:HB2	1:L:388:GLU:CD	2.45	0.42
1:M:60:VAL:HG23	1:M:67:TRP:CD2	2.55	0.42
1:N:285:LEU:HD13	1:N:341:PHE:CE2	2.55	0.42
1:R:31:LEU:O	1:R:35:ILE:HG13	2.19	0.42
1:R:326:ALA:O	1:R:328:ILE:HG23	2.18	0.42
1:A:424:TYR:HA	1:A:425:PRO:HD3	1.86	0.42
1:B:469:ASP:OD2	1:B:471:GLU:HG2	2.20	0.42
1:H:219:GLN:NE2	2:H:515:HOH:O	2.53	0.42
1:J:218:ASN:HB2	1:J:247:MET:HE3	2.02	0.42
1:K:67:TRP:CE3	1:K:182:LYS:HG3	2.55	0.42
1:K:241:ALA:O	1:K:245:ARG:HD2	2.20	0.42
1:L:178:PHE:CE1	1:L:182:LYS:HE3	2.55	0.42
1:L:391:ASP:C	1:L:393:ASN:N	2.77	0.42
1:M:219:GLN:O	1:M:223:LYS:HG2	2.19	0.42
1:O:133:GLU:HA	1:O:323:ARG:HD2	2.01	0.42
1:O:278:PRO:HG2	1:O:281:MET:SD	2.60	0.42
1:Q:37:GLY:O	1:Q:38:LEU:HD12	2.20	0.42
1:R:312:ILE:O	1:R:316:SER:HB3	2.19	0.42
1:B:15:ARG:HD2	1:B:396:TYR:CD2	2.54	0.42
1:H:407:GLN:HA	1:H:412:GLN:HE21	1.84	0.42
1:K:219:GLN:H	1:K:219:GLN:HG3	1.72	0.42
1:L:279:ARG:H	1:L:279:ARG:HG2	1.50	0.42
1:C:16:ILE:N	2:C:513:HOH:O	2.37	0.42
1:G:441:VAL:HG13	1:G:456:VAL:HB	2.02	0.42
1:H:263:LEU:HD23	1:H:263:LEU:HA	1.86	0.42
1:H:399:LEU:O	1:H:403:GLU:HG2	2.19	0.42
1:I:223:LYS:HB3	1:I:223:LYS:HE2	1.51	0.42
1:K:430:HIS:CE1	1:K:446:ARG:HB3	2.54	0.42
1:M:15:ARG:HG2	1:M:370:TYR:OH	2.20	0.42
1:N:15:ARG:HA	1:N:15:ARG:HD3	1.77	0.42
1:P:88:ILE:HD11	1:P:111:PHE:HE1	1.83	0.42
1:Q:110:LEU:HD11	1:Q:161:LEU:HD22	2.02	0.42
1:B:1:MET:HE2	1:B:2:LEU:H	1.85	0.42
1:B:18:ASN:O	1:K:63:LYS:HE3	2.19	0.42
1:B:450:TYR:HE1	1:B:470:VAL:HG12	1.85	0.42
1:E:80:CYS:HA	1:E:186:LEU:O	2.20	0.42
1:E:286:ASP:OD1	1:E:286:ASP:N	2.53	0.42
1:F:79:LEU:HD23	1:F:184:VAL:HG12	2.02	0.42
1:G:38:LEU:HD23	1:G:38:LEU:HA	1.85	0.42
1:H:395:HIS:NE2	1:H:396:TYR:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:LYS:H	1:I:134:LYS:HG2	1.53	0.42
1:J:454:LEU:HD11	1:J:456:VAL:HG23	2.01	0.42
1:L:390:ARG:HD2	1:L:394:ARG:NH2	2.35	0.42
1:N:82:ASP:OD2	1:N:188:ARG:HD3	2.19	0.42
1:N:132:LYS:HE3	1:N:134:LYS:HD3	2.00	0.42
1:P:214:LEU:HD22	1:P:247:MET:HE1	2.02	0.42
1:Q:87:HIS:CD2	1:Q:158:GLN:HG2	2.55	0.42
1:R:79:LEU:HD23	1:R:79:LEU:HA	1.86	0.42
1:C:233:HIS:HA	1:C:295:ASP:OD2	2.20	0.41
1:E:39:HIS:HD2	2:E:501:HOH:O	2.02	0.41
1:E:324:SER:O	1:E:325:ALA:HB3	2.20	0.41
1:I:273:TRP:CH2	1:I:281:MET:HE1	2.55	0.41
1:P:63:LYS:HE2	1:P:63:LYS:HB3	1.96	0.41
1:P:421:ARG:HA	1:P:427:PHE:CE2	2.55	0.41
1:A:267:SER:O	1:A:271:LYS:HG3	2.20	0.41
1:C:207:GLU:HG2	1:C:211:TYR:CE2	2.55	0.41
1:C:236:THR:HG22	2:C:591:HOH:O	2.20	0.41
1:C:240:TYR:CZ	1:C:278:PRO:HG3	2.54	0.41
1:C:383:MET:HE3	1:C:383:MET:HB3	1.66	0.41
1:C:431:PHE:HB2	1:C:445:TRP:CH2	2.55	0.41
1:F:218:ASN:O	1:F:222:LEU:HD13	2.20	0.41
1:I:103:PHE:CZ	1:I:148:THR:HG21	2.54	0.41
1:J:409:PRO:O	1:J:413:ARG:HG3	2.21	0.41
1:K:301:PRO:O	1:K:305:ILE:HG13	2.19	0.41
1:P:162:ASN:ND2	1:P:165:SER:HB3	2.34	0.41
1:R:15:ARG:HD3	1:R:15:ARG:HA	1.28	0.41
1:A:382:LEU:HG	1:A:391:ASP:HB3	2.02	0.41
1:B:42:PRO:HD3	1:B:82:ASP:OD1	2.19	0.41
1:B:244:ARG:NH1	1:B:244:ARG:HG3	2.35	0.41
1:B:478:LEU:HD22	1:B:479:GLU:H	1.85	0.41
1:G:349:ASP:OD1	1:G:349:ASP:N	2.53	0.41
1:H:4:LYS:HG3	1:H:78:ASP:OD2	2.21	0.41
1:M:389:LEU:O	1:M:392:ILE:HB	2.20	0.41
1:O:293:ILE:N	1:O:294:PRO:HD2	2.35	0.41
1:P:44:PHE:HB3	1:P:56:THR:O	2.20	0.41
1:P:400:GLU:O	1:P:404:GLN:HG2	2.21	0.41
1:R:85:VAL:HA	1:R:172:MET:HE3	2.02	0.41
1:R:120:ILE:HG22	1:R:125:MET:HG2	2.02	0.41
1:B:22:ASP:HB3	1:B:399:LEU:HD21	2.03	0.41
1:D:286:ASP:OD1	1:D:369:TYR:HB3	2.20	0.41
1:E:256:PRO:HG2	1:E:296:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ILE:HD11	1:F:367:GLN:HB3	2.02	0.41
1:F:272:ASN:O	1:F:276:MET:HG2	2.20	0.41
1:H:142:LEU:HD12	1:H:146:THR:HB	2.02	0.41
1:I:130:ILE:HG13	1:I:323:ARG:HH22	1.85	0.41
1:I:215:ASP:O	1:I:219:GLN:HG2	2.20	0.41
1:K:9:LEU:HD13	1:K:373:LEU:HD22	2.02	0.41
1:K:339:CYS:SG	1:K:344:ALA:HB2	2.60	0.41
1:K:464:LYS:HE3	1:K:477:HIS:CE1	2.55	0.41
1:L:80:CYS:HA	1:L:186:LEU:O	2.20	0.41
1:O:228:CYS:HB2	1:O:247:MET:HG2	2.03	0.41
1:R:235:HIS:HA	2:R:507:HOH:O	2.20	0.41
1:A:272:ASN:O	1:A:276:MET:HG2	2.21	0.41
1:D:209:GLU:H	1:D:209:GLU:CD	2.27	0.41
1:G:258:LEU:HA	1:G:258:LEU:HD23	1.78	0.41
1:G:375:ALA:HB3	1:G:408:LYS:NZ	2.35	0.41
1:J:293:ILE:O	1:J:296:VAL:HG12	2.20	0.41
1:L:285:LEU:HB2	1:L:356:ARG:NH1	2.35	0.41
1:M:141:THR:HG21	1:M:147:LYS:HE2	2.02	0.41
1:O:210:VAL:HA	1:O:213:ILE:HD12	2.03	0.41
1:O:379:ASP:CG	1:O:382:LEU:HB2	2.45	0.41
1:Q:346:MET:HE3	1:Q:346:MET:HB2	1.87	0.41
1:R:82:ASP:HA	1:R:188:ARG:HB3	2.03	0.41
1:R:312:ILE:HG21	1:R:337:LEU:HD13	2.01	0.41
1:R:348:ASN:HB3	1:R:351:ALA:HB3	2.03	0.41
1:C:132:LYS:NZ	1:C:152:CYS:O	2.51	0.41
1:C:141:THR:HG23	1:C:147:LYS:HD2	2.01	0.41
1:D:417:LEU:HD23	1:D:417:LEU:HA	1.94	0.41
1:E:400:GLU:HG3	1:E:401:GLU:N	2.33	0.41
1:G:34:ALA:HB1	1:G:418:MET:HE2	2.03	0.41
1:I:3:LEU:HD11	1:I:186:LEU:HD13	2.01	0.41
1:L:391:ASP:O	1:L:392:ILE:C	2.63	0.41
1:M:476:ARG:HE	1:M:476:ARG:HB3	1.67	0.41
1:P:327:ASN:ND2	1:P:330:SER:HB3	2.35	0.41
1:Q:302:ASP:OD2	1:Q:331:VAL:HG21	2.20	0.41
1:C:255:PRO:HG2	1:C:256:PRO:HD3	2.02	0.41
1:G:63:LYS:H	1:G:63:LYS:HG2	1.75	0.41
1:G:80:CYS:HB2	1:G:186:LEU:HD23	2.03	0.41
1:K:255:PRO:HB2	1:K:256:PRO:HD3	2.02	0.41
1:L:327:ASN:OD1	1:L:330:SER:HB3	2.20	0.41
1:M:398:THR:HG23	1:M:401:GLU:CD	2.45	0.41
1:N:23:LEU:O	1:N:27:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:67:TRP:CD2	1:N:182:LYS:HD2	2.56	0.41
1:O:340:THR:HG22	1:O:393:ASN:OD1	2.20	0.41
1:O:424:TYR:CE2	1:O:452:CYS:HB3	2.55	0.41
1:P:388:GLU:HB3	1:P:391:ASP:OD2	2.21	0.41
1:Q:17:GLY:O	2:Q:501:HOH:O	2.22	0.41
1:R:292:CYS:SG	1:R:294:PRO:HD2	2.61	0.41
1:R:390:ARG:HH21	1:R:394:ARG:HH22	1.69	0.41
1:A:125:MET:HA	1:A:128:ILE:HD12	2.03	0.41
1:A:142:LEU:HD12	1:A:146:THR:OG1	2.21	0.41
1:G:87:HIS:CD2	1:G:158:GLN:HG2	2.55	0.41
1:L:383:MET:HE3	1:L:383:MET:HB3	1.68	0.41
1:M:407:GLN:O	1:M:408:LYS:C	2.63	0.41
1:N:112:VAL:HG13	1:N:151:TRP:HB3	2.02	0.41
1:N:218:ASN:HB2	1:N:247:MET:HE3	2.03	0.41
1:P:61:ASP:O	1:P:64:VAL:HG22	2.21	0.41
1:P:180:THR:HG21	1:P:224:HIS:CB	2.51	0.41
1:Q:331:VAL:HG23	1:Q:332:GLY:H	1.85	0.41
1:B:424:TYR:HA	1:B:425:PRO:HD3	1.81	0.41
1:C:53:SER:O	1:C:89:SER:HB2	2.21	0.41
1:D:112:VAL:HG22	1:D:162:ASN:HB2	2.03	0.41
1:G:47:ASN:ND2	1:G:91:GLU:HB2	2.35	0.41
1:H:4:LYS:HG3	1:H:4:LYS:H	1.70	0.41
1:H:244:ARG:HH11	1:H:244:ARG:HD3	1.63	0.41
1:I:222:LEU:HD12	1:I:222:LEU:HA	1.83	0.41
1:J:113:HIS:HB3	2:J:553:HOH:O	2.20	0.41
1:J:219:GLN:HG3	1:J:220:VAL:N	2.34	0.41
1:J:340:THR:HG22	1:J:393:ASN:OD1	2.20	0.41
1:J:466:THR:HA	1:J:476:ARG:O	2.21	0.41
1:M:141:THR:HG22	1:M:147:LYS:HE2	2.02	0.41
1:M:286:ASP:OD2	1:M:369:TYR:HB3	2.20	0.41
1:M:380:HIS:HA	1:M:383:MET:HE2	2.02	0.41
1:N:67:TRP:HZ3	1:N:70:ILE:HG21	1.85	0.41
1:N:153:THR:HG21	1:N:194:TYR:CD1	2.56	0.41
1:N:392:ILE:HG12	1:N:393:ASN:N	2.32	0.41
1:O:9:LEU:HD13	1:O:373:LEU:HD22	2.02	0.41
1:O:327:ASN:HD22	1:O:330:SER:HB2	1.86	0.41
1:P:67:TRP:CE3	1:P:182:LYS:HG3	2.55	0.41
1:P:130:ILE:O	1:P:323:ARG:NH2	2.50	0.41
1:P:380:HIS:HA	1:P:383:MET:HE3	2.02	0.41
1:Q:97:ASP:HB3	1:Q:107:TYR:HD2	1.86	0.41
1:R:49:ASP:HB3	1:R:52:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:388:GLU:HG3	1:R:391:ASP:H	1.86	0.41
1:R:415:LEU:HD23	1:R:415:LEU:HA	1.93	0.41
1:A:10:ILE:HG12	1:A:369:TYR:CD1	2.51	0.41
1:E:75:ALA:HB1	1:N:220:VAL:HA	2.03	0.41
1:F:39:HIS:HA	1:F:80:CYS:O	2.20	0.41
1:F:144:ASP:OD1	1:F:146:THR:OG1	2.31	0.41
1:F:267:SER:O	1:F:271:LYS:HG3	2.21	0.41
1:H:130:ILE:O	1:H:130:ILE:HD12	2.20	0.41
1:H:323:ARG:HE	1:H:323:ARG:HB3	1.68	0.41
1:K:219:GLN:O	1:K:223:LYS:HG2	2.21	0.41
1:L:286:ASP:CG	1:L:369:TYR:HB3	2.46	0.41
1:M:302:ASP:CG	1:M:331:VAL:HG21	2.45	0.41
1:M:383:MET:HG3	1:M:388:GLU:O	2.20	0.41
1:N:479:GLU:H	1:N:479:GLU:HG2	1.39	0.41
1:O:58:LYS:HD3	1:O:178:PHE:CD2	2.56	0.41
1:R:216:TRP:CH2	1:R:220:VAL:HG21	2.56	0.41
1:R:391:ASP:HA	1:R:394:ARG:CG	2.51	0.41
1:R:450:TYR:CE2	1:R:470:VAL:HG13	2.55	0.41
1:B:214:LEU:HD12	1:B:214:LEU:HA	1.71	0.40
1:D:480:CYS:HB2	2:D:572:HOH:O	2.21	0.40
1:F:213:ILE:O	1:F:217:VAL:HG13	2.21	0.40
1:F:319:PRO:HG2	1:F:321:MET:HE1	2.02	0.40
1:H:82:ASP:OD2	1:H:188:ARG:HD3	2.21	0.40
1:H:140:VAL:HA	2:H:531:HOH:O	2.21	0.40
1:I:124:ASP:OD2	2:I:502:HOH:O	2.21	0.40
1:K:55:LEU:O	2:K:502:HOH:O	2.22	0.40
1:K:285:LEU:HD12	1:K:285:LEU:HA	1.94	0.40
1:L:100:ALA:HA	1:L:143:SER:HB2	2.04	0.40
1:N:134:LYS:HG2	1:N:135:GLU:O	2.21	0.40
1:O:99:ILE:HD11	1:O:140:VAL:CG1	2.51	0.40
1:P:134:LYS:HB3	1:P:134:LYS:HE2	1.56	0.40
1:P:258:LEU:HD22	1:P:262:LEU:HD11	2.02	0.40
1:Q:303:GLU:H	1:Q:303:GLU:HG3	1.61	0.40
1:R:229:LEU:HD21	1:R:250:TYR:CZ	2.54	0.40
1:R:454:LEU:HD11	1:R:456:VAL:HG23	2.04	0.40
1:B:306:LYS:HG3	1:B:331:VAL:HG12	2.02	0.40
1:D:117:PHE:HB3	1:D:199:ILE:HG13	2.03	0.40
1:D:132:LYS:NZ	1:D:154:PHE:O	2.54	0.40
1:F:328:ILE:H	1:F:328:ILE:HG13	1.54	0.40
1:G:79:LEU:HD12	1:G:79:LEU:HA	1.89	0.40
1:G:349:ASP:OD2	1:G:410:VAL:HB	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:350:ASP:HB3	1:G:461:LYS:O	2.21	0.40
1:I:125:MET:HE1	1:I:137:PHE:HZ	1.86	0.40
1:K:90:ASP:N	1:K:157:GLN:O	2.52	0.40
1:K:180:THR:HG21	1:K:224:HIS:HB3	2.03	0.40
1:L:108:ALA:O	1:L:113:HIS:HE1	2.04	0.40
1:L:134:LYS:H	1:L:134:LYS:HG2	1.63	0.40
1:L:244:ARG:HG3	1:L:244:ARG:NH1	2.35	0.40
1:L:272:ASN:O	1:L:276:MET:HG2	2.22	0.40
1:L:431:PHE:HB2	1:L:445:TRP:CZ2	2.56	0.40
1:M:2:LEU:HD13	1:M:227:GLU:OE2	2.21	0.40
1:M:115:ASP:O	1:M:116:LYS:C	2.64	0.40
1:Q:383:MET:HG3	1:Q:388:GLU:O	2.21	0.40
1:Q:404:GLN:HG2	1:Q:404:GLN:H	1.60	0.40
1:C:249:PRO:HG2	1:C:281:MET:HB2	2.03	0.40
1:C:471:GLU:H	1:C:471:GLU:HG3	1.47	0.40
1:E:81:VAL:HG21	1:E:179:LEU:HD22	2.04	0.40
1:F:300:LEU:HD23	1:F:300:LEU:HA	1.92	0.40
1:G:285:LEU:HD23	1:G:285:LEU:HA	1.86	0.40
1:I:242:ILE:HG23	1:I:247:MET:HB2	2.03	0.40
1:I:456:VAL:HG22	1:I:463:VAL:HG22	2.03	0.40
1:I:469:ASP:HB3	1:I:473:GLY:H	1.86	0.40
1:J:426:ALA:HA	1:J:447:HIS:HB3	2.03	0.40
1:K:285:LEU:HD21	1:K:355:ALA:HB1	2.04	0.40
1:N:90:ASP:HB3	1:N:159:ILE:HD11	2.04	0.40
1:N:214:LEU:HD23	1:N:214:LEU:HA	1.93	0.40
1:N:242:ILE:HG23	1:N:247:MET:HB2	2.03	0.40
1:O:15:ARG:HD2	1:O:396:TYR:CD2	2.57	0.40
1:R:286:ASP:HB3	1:R:341:PHE:HB2	2.03	0.40
1:R:380:HIS:HA	1:R:392:ILE:CD1	2.52	0.40
1:A:274:LEU:HD13	1:A:443:MET:HE3	2.02	0.40
1:C:380:HIS:CE1	1:C:392:ILE:HD11	2.57	0.40
1:F:182:LYS:HA	1:F:182:LYS:HD2	1.77	0.40
1:G:223:LYS:HG3	1:G:224:HIS:N	2.36	0.40
1:G:356:ARG:NH1	1:G:368:VAL:HG22	2.37	0.40
1:J:86:ASN:HB3	1:J:87:HIS:ND1	2.36	0.40
1:K:380:HIS:O	1:K:384:GLU:HG2	2.21	0.40
1:O:123:ASP:O	1:O:127:LYS:HG3	2.22	0.40
1:O:397:TYR:HA	1:O:401:GLU:OE1	2.21	0.40
1:P:12:TYR:CZ	1:P:41:LEU:HD22	2.56	0.40
1:P:390:ARG:HB3	1:P:394:ARG:HD2	2.03	0.40
1:Q:413:ARG:NH2	1:Q:480:CYS:OXT	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:321:MET:HE3	1:R:321:MET:HB3	1.79	0.40
1:B:12:TYR:CG	1:B:15:ARG:HG2	2.56	0.40
1:B:192:PHE:HE2	1:B:232:VAL:HG22	1.85	0.40
1:B:461:LYS:NZ	1:G:133:GLU:OE1	2.52	0.40
1:H:76:LYS:HB2	1:H:76:LYS:HE2	1.86	0.40
1:I:80:CYS:HA	1:I:186:LEU:O	2.21	0.40
1:K:322:ARG:HG3	1:K:332:GLY:O	2.21	0.40
1:M:138:ARG:NH1	1:M:156:GLU:O	2.54	0.40
1:M:441:VAL:HG22	1:M:456:VAL:HB	2.04	0.40
1:O:41:LEU:HD13	1:O:41:LEU:HA	1.89	0.40
1:O:247:MET:HE2	1:O:247:MET:HB2	1.63	0.40
1:O:308:LEU:O	1:O:312:ILE:HG12	2.21	0.40
1:P:325:ALA:CB	1:P:333:ALA:HA	2.51	0.40
1:P:471:GLU:H	1:P:471:GLU:HG3	1.54	0.40
1:Q:15:ARG:HD3	1:Q:396:TYR:CE2	2.56	0.40
1:Q:402:VAL:O	1:Q:406:ILE:HG12	2.22	0.40
1:R:22:ASP:O	1:R:26:VAL:HG13	2.20	0.40
1:R:131:ARG:HD3	1:R:322:ARG:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/480 (100%)	465 (97%)	13 (3%)	0	100	100
1	B	478/480 (100%)	464 (97%)	14 (3%)	0	100	100
1	C	478/480 (100%)	468 (98%)	10 (2%)	0	100	100
1	D	478/480 (100%)	469 (98%)	9 (2%)	0	100	100
1	E	477/480 (99%)	464 (97%)	13 (3%)	0	100	100
1	F	478/480 (100%)	464 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	477/480 (99%)	463 (97%)	14 (3%)	0	100	100
1	H	478/480 (100%)	466 (98%)	12 (2%)	0	100	100
1	I	478/480 (100%)	467 (98%)	11 (2%)	0	100	100
1	J	478/480 (100%)	462 (97%)	16 (3%)	0	100	100
1	K	478/480 (100%)	468 (98%)	10 (2%)	0	100	100
1	L	478/480 (100%)	467 (98%)	11 (2%)	0	100	100
1	M	478/480 (100%)	462 (97%)	16 (3%)	0	100	100
1	N	478/480 (100%)	465 (97%)	13 (3%)	0	100	100
1	O	478/480 (100%)	467 (98%)	11 (2%)	0	100	100
1	P	478/480 (100%)	466 (98%)	12 (2%)	0	100	100
1	Q	478/480 (100%)	463 (97%)	15 (3%)	0	100	100
1	R	478/480 (100%)	466 (98%)	12 (2%)	0	100	100
All	All	8602/8640 (100%)	8376 (97%)	226 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	426/426 (100%)	403 (95%)	23 (5%)	20	35
1	B	426/426 (100%)	403 (95%)	23 (5%)	20	35
1	C	426/426 (100%)	406 (95%)	20 (5%)	23	41
1	D	426/426 (100%)	399 (94%)	27 (6%)	16	29
1	E	425/426 (100%)	401 (94%)	24 (6%)	19	33
1	F	424/426 (100%)	396 (93%)	28 (7%)	15	26
1	G	425/426 (100%)	391 (92%)	34 (8%)	11	19
1	H	426/426 (100%)	390 (92%)	36 (8%)	10	16
1	I	426/426 (100%)	394 (92%)	32 (8%)	12	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	426/426 (100%)	390 (92%)	36 (8%)	10	16
1	K	426/426 (100%)	387 (91%)	39 (9%)	8	14
1	L	426/426 (100%)	380 (89%)	46 (11%)	6	9
1	M	426/426 (100%)	390 (92%)	36 (8%)	10	16
1	N	426/426 (100%)	391 (92%)	35 (8%)	10	18
1	O	426/426 (100%)	385 (90%)	41 (10%)	8	12
1	P	426/426 (100%)	380 (89%)	46 (11%)	6	9
1	Q	426/426 (100%)	403 (95%)	23 (5%)	20	35
1	R	426/426 (100%)	380 (89%)	46 (11%)	6	9
All	All	7664/7668 (100%)	7069 (92%)	595 (8%)	11	20

All (595) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	ARG
1	A	18	ASN
1	A	41	LEU
1	A	71	GLU
1	A	119	GLU
1	A	152	CYS
1	A	155	THR
1	A	214	LEU
1	A	232	VAL
1	A	324	SER
1	A	381	GLU
1	A	385	GLN
1	A	388	GLU
1	A	390	ARG
1	A	400	GLU
1	A	407	GLN
1	A	416	SER
1	A	439	SER
1	A	471	GLU
1	A	476	ARG
1	A	478	LEU
1	A	479	GLU
1	B	1	MET
1	B	2	LEU

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Mol	Chain	Res	Type
1	B	35	ILE
1	B	131	ARG
1	B	152	CYS
1	B	156	GLU
1	B	196	THR
1	B	214	LEU
1	B	231	GLU
1	B	232	VAL
1	B	286	ASP
1	B	304	LYS
1	B	312	ILE
1	B	327	ASN
1	B	331	VAL
1	B	339	CYS
1	B	384	GLU
1	B	400	GLU
1	B	471	GLU
1	B	472	THR
1	B	478	LEU
1	B	479	GLU
1	B	480	CYS
1	C	15	ARG
1	C	41	LEU
1	C	70	ILE
1	C	76	LYS
1	C	105	SER
1	C	152	CYS
1	C	236	THR
1	C	279	ARG
1	C	281	MET
1	C	338	THR
1	C	381	GLU
1	C	383	MET
1	C	385	GLN
1	C	416	SER
1	C	439	SER
1	C	469	ASP
1	C	471	GLU
1	C	474	GLU
1	C	476	ARG
1	C	478	LEU
1	D	15	ARG

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Mol	Chain	Res	Type
1	D	41	LEU
1	D	64	VAL
1	D	70	ILE
1	D	76	LYS
1	D	81	VAL
1	D	138	ARG
1	D	140	VAL
1	D	165	SER
1	D	201	THR
1	D	232	VAL
1	D	243	SER
1	D	279	ARG
1	D	281	MET
1	D	302	ASP
1	D	338	THR
1	D	343	ASP
1	D	374	LEU
1	D	381	GLU
1	D	385	GLN
1	D	407	GLN
1	D	408	LYS
1	D	416	SER
1	D	441	VAL
1	D	471	GLU
1	D	476	ARG
1	D	479	GLU
1	E	15	ARG
1	E	39	HIS
1	E	41	LEU
1	E	76	LYS
1	E	134	LYS
1	E	140	VAL
1	E	144	ASP
1	E	148	THR
1	E	152	CYS
1	E	197	LYS
1	E	222	LEU
1	E	223	LYS
1	E	231	GLU
1	E	279	ARG
1	E	281	MET
1	E	308	LEU

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Mol	Chain	Res	Type
1	E	386	SER
1	E	390	ARG
1	E	392	ILE
1	E	398	THR
1	E	400	GLU
1	E	403	GLU
1	E	404	GLN
1	E	439	SER
1	F	38	LEU
1	F	41	LEU
1	F	76	LYS
1	F	81	VAL
1	F	119	GLU
1	F	130	ILE
1	F	131	ARG
1	F	132	LYS
1	F	134	LYS
1	F	185	ASN
1	F	215	ASP
1	F	217	VAL
1	F	231	GLU
1	F	279	ARG
1	F	285	LEU
1	F	296	VAL
1	F	302	ASP
1	F	303	GLU
1	F	304	LYS
1	F	306	LYS
1	F	328	ILE
1	F	381	GLU
1	F	382	LEU
1	F	385	GLN
1	F	390	ARG
1	F	404	GLN
1	F	441	VAL
1	F	479	GLU
1	G	41	LEU
1	G	58	LYS
1	G	70	ILE
1	G	76	LYS
1	G	116	LYS
1	G	123	ASP

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Mol	Chain	Res	Type
1	G	140	VAL
1	G	147	LYS
1	G	148	THR
1	G	173	GLU
1	G	184	VAL
1	G	185	ASN
1	G	219	GLN
1	G	222	LEU
1	G	223	LYS
1	G	227	GLU
1	G	232	VAL
1	G	236	THR
1	G	279	ARG
1	G	281	MET
1	G	330	SER
1	G	343	ASP
1	G	392	ILE
1	G	400	GLU
1	G	417	LEU
1	G	419	LYS
1	G	439	SER
1	G	441	VAL
1	G	449	ASP
1	G	470	VAL
1	G	475	THR
1	G	476	ARG
1	G	478	LEU
1	G	479	GLU
1	H	15	ARG
1	H	30	HIS
1	H	35	ILE
1	H	38	LEU
1	H	39	HIS
1	H	64	VAL
1	H	71	GLU
1	H	76	LYS
1	H	130	ILE
1	H	131	ARG
1	H	133	GLU
1	H	140	VAL
1	H	152	CYS
1	H	174	SER

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Mol	Chain	Res	Type
1	H	231	GLU
1	H	279	ARG
1	H	280	ASN
1	H	281	MET
1	H	303	GLU
1	H	324	SER
1	H	331	VAL
1	H	343	ASP
1	H	383	MET
1	H	385	GLN
1	H	390	ARG
1	H	392	ILE
1	H	400	GLU
1	H	407	GLN
1	H	408	LYS
1	H	439	SER
1	H	464	LYS
1	H	466	THR
1	H	470	VAL
1	H	471	GLU
1	H	472	THR
1	H	478	LEU
1	I	10	ILE
1	I	70	ILE
1	I	76	LYS
1	I	115	ASP
1	I	130	ILE
1	I	133	GLU
1	I	134	LYS
1	I	142	LEU
1	I	152	CYS
1	I	154	PHE
1	I	165	SER
1	I	222	LEU
1	I	223	LYS
1	I	231	GLU
1	I	236	THR
1	I	239	GLN
1	I	244	ARG
1	I	245	ARG
1	I	247	MET
1	I	302	ASP

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Mol	Chain	Res	Type
1	I	303	GLU
1	I	304	LYS
1	I	321	MET
1	I	323	ARG
1	I	381	GLU
1	I	383	MET
1	I	389	LEU
1	I	392	ILE
1	I	394	ARG
1	I	400	GLU
1	I	464	LYS
1	I	478	LEU
1	J	21	LYS
1	J	41	LEU
1	J	76	LYS
1	J	101	ASN
1	J	105	SER
1	J	121	SER
1	J	133	GLU
1	J	134	LYS
1	J	184	VAL
1	J	196	THR
1	J	219	GLN
1	J	231	GLU
1	J	245	ARG
1	J	279	ARG
1	J	280	ASN
1	J	281	MET
1	J	302	ASP
1	J	303	GLU
1	J	304	LYS
1	J	307	VAL
1	J	309	ILE
1	J	330	SER
1	J	343	ASP
1	J	374	LEU
1	J	381	GLU
1	J	384	GLU
1	J	388	GLU
1	J	389	LEU
1	J	400	GLU
1	J	415	LEU

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Mol	Chain	Res	Type
1	J	416	SER
1	J	439	SER
1	J	471	GLU
1	J	476	ARG
1	J	478	LEU
1	J	480	CYS
1	K	25	THR
1	K	35	ILE
1	K	38	LEU
1	K	40	ILE
1	K	41	LEU
1	K	74	THR
1	K	76	LYS
1	K	109	ASP
1	K	127	LYS
1	K	129	HIS
1	K	131	ARG
1	K	133	GLU
1	K	135	GLU
1	K	140	VAL
1	K	147	LYS
1	K	149	ARG
1	K	152	CYS
1	K	174	SER
1	K	184	VAL
1	K	185	ASN
1	K	219	GLN
1	K	222	LEU
1	K	231	GLU
1	K	279	ARG
1	K	281	MET
1	K	302	ASP
1	K	306	LYS
1	K	307	VAL
1	K	322	ARG
1	K	323	ARG
1	K	330	SER
1	K	343	ASP
1	K	374	LEU
1	K	381	GLU
1	K	385	GLN
1	K	400	GLU

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Mol	Chain	Res	Type
1	K	432	GLU
1	K	439	SER
1	K	464	LYS
1	L	2	LEU
1	L	33	GLU
1	L	38	LEU
1	L	41	LEU
1	L	63	LYS
1	L	66	THR
1	L	71	GLU
1	L	76	LYS
1	L	84	THR
1	L	105	SER
1	L	106	GLU
1	L	109	ASP
1	L	119	GLU
1	L	121	SER
1	L	128	ILE
1	L	131	ARG
1	L	133	GLU
1	L	134	LYS
1	L	147	LYS
1	L	149	ARG
1	L	165	SER
1	L	184	VAL
1	L	185	ASN
1	L	219	GLN
1	L	222	LEU
1	L	223	LYS
1	L	234	ASP
1	L	279	ARG
1	L	280	ASN
1	L	281	MET
1	L	321	MET
1	L	323	ARG
1	L	337	LEU
1	L	381	GLU
1	L	383	MET
1	L	388	GLU
1	L	392	ILE
1	L	398	THR
1	L	400	GLU

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Mol	Chain	Res	Type
1	L	406	ILE
1	L	430	HIS
1	L	432	GLU
1	L	433	LEU
1	L	468	THR
1	L	471	GLU
1	L	479	GLU
1	M	31	LEU
1	M	32	SER
1	M	41	LEU
1	M	66	THR
1	M	71	GLU
1	M	76	LYS
1	M	106	GLU
1	M	130	ILE
1	M	131	ARG
1	M	133	GLU
1	M	140	VAL
1	M	166	ASP
1	M	173	GLU
1	M	196	THR
1	M	232	VAL
1	M	258	LEU
1	M	281	MET
1	M	287	THR
1	M	296	VAL
1	M	302	ASP
1	M	304	LYS
1	M	315	ARG
1	M	322	ARG
1	M	338	THR
1	M	385	GLN
1	M	390	ARG
1	M	392	ILE
1	M	398	THR
1	M	400	GLU
1	M	404	GLN
1	M	408	LYS
1	M	439	SER
1	M	471	GLU
1	M	474	GLU
1	M	476	ARG

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Mol	Chain	Res	Type
1	M	480	CYS
1	N	15	ARG
1	N	25	THR
1	N	41	LEU
1	N	69	ASP
1	N	70	ILE
1	N	76	LYS
1	N	81	VAL
1	N	89	SER
1	N	105	SER
1	N	130	ILE
1	N	131	ARG
1	N	133	GLU
1	N	134	LYS
1	N	139	GLU
1	N	154	PHE
1	N	180	THR
1	N	245	ARG
1	N	279	ARG
1	N	280	ASN
1	N	302	ASP
1	N	303	GLU
1	N	306	LYS
1	N	307	VAL
1	N	321	MET
1	N	324	SER
1	N	390	ARG
1	N	392	ILE
1	N	398	THR
1	N	401	GLU
1	N	404	GLN
1	N	408	LYS
1	N	449	ASP
1	N	466	THR
1	N	479	GLU
1	N	480	CYS
1	O	14	ASP
1	O	15	ARG
1	O	21	LYS
1	O	35	ILE
1	O	38	LEU
1	O	41	LEU

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Mol	Chain	Res	Type
1	O	66	THR
1	O	69	ASP
1	O	70	ILE
1	O	76	LYS
1	O	96	THR
1	O	132	LYS
1	O	134	LYS
1	O	137	PHE
1	O	155	THR
1	O	164	GLU
1	O	165	SER
1	O	196	THR
1	O	197	LYS
1	O	201	THR
1	O	247	MET
1	O	280	ASN
1	O	281	MET
1	O	313	ASP
1	O	321	MET
1	O	322	ARG
1	O	331	VAL
1	O	381	GLU
1	O	384	GLU
1	O	388	GLU
1	O	391	ASP
1	O	398	THR
1	O	400	GLU
1	O	404	GLN
1	O	439	SER
1	O	441	VAL
1	O	468	THR
1	O	471	GLU
1	O	475	THR
1	O	476	ARG
1	O	479	GLU
1	P	1	MET
1	P	2	LEU
1	P	4	LYS
1	P	25	THR
1	P	28	ASP
1	P	76	LYS
1	P	81	VAL

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Mol	Chain	Res	Type
1	P	112	VAL
1	P	115	ASP
1	P	119	GLU
1	P	123	ASP
1	P	131	ARG
1	P	132	LYS
1	P	133	GLU
1	P	134	LYS
1	P	139	GLU
1	P	144	ASP
1	P	146	THR
1	P	147	LYS
1	P	148	THR
1	P	149	ARG
1	P	153	THR
1	P	165	SER
1	P	167	LEU
1	P	182	LYS
1	P	222	LEU
1	P	258	LEU
1	P	279	ARG
1	P	302	ASP
1	P	322	ARG
1	P	378	ASN
1	P	381	GLU
1	P	382	LEU
1	P	383	MET
1	P	385	GLN
1	P	390	ARG
1	P	392	ILE
1	P	398	THR
1	P	416	SER
1	P	419	LYS
1	P	439	SER
1	P	441	VAL
1	P	470	VAL
1	P	475	THR
1	P	476	ARG
1	P	479	GLU
1	Q	9	LEU
1	Q	41	LEU
1	Q	64	VAL

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Mol	Chain	Res	Type
1	Q	76	LYS
1	Q	106	GLU
1	Q	119	GLU
1	Q	140	VAL
1	Q	152	CYS
1	Q	184	VAL
1	Q	227	GLU
1	Q	231	GLU
1	Q	236	THR
1	Q	302	ASP
1	Q	303	GLU
1	Q	315	ARG
1	Q	323	ARG
1	Q	338	THR
1	Q	385	GLN
1	Q	389	LEU
1	Q	400	GLU
1	Q	404	GLN
1	Q	474	GLU
1	Q	480	CYS
1	R	15	ARG
1	R	26	VAL
1	R	27	VAL
1	R	35	ILE
1	R	39	HIS
1	R	40	ILE
1	R	56	THR
1	R	59	GLU
1	R	63	LYS
1	R	64	VAL
1	R	66	THR
1	R	76	LYS
1	R	79	LEU
1	R	82	ASP
1	R	89	SER
1	R	130	ILE
1	R	131	ARG
1	R	133	GLU
1	R	152	CYS
1	R	156	GLU
1	R	161	LEU
1	R	165	SER

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Mol	Chain	Res	Type
1	R	174	SER
1	R	184	VAL
1	R	189	LEU
1	R	231	GLU
1	R	236	THR
1	R	258	LEU
1	R	279	ARG
1	R	280	ASN
1	R	296	VAL
1	R	307	VAL
1	R	313	ASP
1	R	328	ILE
1	R	330	SER
1	R	381	GLU
1	R	385	GLN
1	R	389	LEU
1	R	399	LEU
1	R	400	GLU
1	R	407	GLN
1	R	408	LYS
1	R	464	LYS
1	R	472	THR
1	R	474	GLU
1	R	476	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	218	ASN
1	A	219	GLN
1	A	266	ASN
1	A	385	GLN
1	A	404	GLN
1	A	423	ASN
1	A	434	ASN
1	B	47	ASN
1	B	129	HIS
1	B	224	HIS
1	B	327	ASN
1	B	434	ASN
1	C	18	ASN

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Mol	Chain	Res	Type
1	C	39	HIS
1	C	219	GLN
1	C	280	ASN
1	C	380	HIS
1	C	412	GLN
1	C	423	ASN
1	D	86	ASN
1	D	87	HIS
1	D	101	ASN
1	D	385	GLN
1	D	430	HIS
1	D	459	ASN
1	E	39	HIS
1	E	162	ASN
1	E	280	ASN
1	E	380	HIS
1	E	393	ASN
1	E	434	ASN
1	E	477	HIS
1	F	86	ASN
1	F	129	HIS
1	F	218	ASN
1	F	266	ASN
1	F	329	HIS
1	F	347	GLN
1	F	380	HIS
1	F	385	GLN
1	F	412	GLN
1	F	423	ASN
1	G	47	ASN
1	G	86	ASN
1	G	87	HIS
1	G	129	HIS
1	G	157	GLN
1	G	162	ASN
1	G	233	HIS
1	G	423	ASN
1	H	18	ASN
1	H	47	ASN
1	H	86	ASN
1	H	129	HIS
1	H	266	ASN

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Mol	Chain	Res	Type
1	H	329	HIS
1	H	385	GLN
1	I	87	HIS
1	I	129	HIS
1	I	218	ASN
1	I	239	GLN
1	I	266	ASN
1	I	434	ASN
1	I	477	HIS
1	J	18	ASN
1	J	30	HIS
1	J	47	ASN
1	J	57	HIS
1	J	86	ASN
1	J	129	HIS
1	J	380	HIS
1	J	407	GLN
1	J	434	ASN
1	K	47	ASN
1	K	219	GLN
1	K	224	HIS
1	K	233	HIS
1	K	246	ASN
1	K	385	GLN
1	K	407	GLN
1	K	423	ASN
1	K	430	HIS
1	L	157	GLN
1	L	162	ASN
1	L	219	GLN
1	L	380	HIS
1	L	385	GLN
1	L	404	GLN
1	M	39	HIS
1	M	86	ASN
1	M	101	ASN
1	M	219	GLN
1	M	224	HIS
1	M	347	GLN
1	M	385	GLN
1	M	395	HIS
1	M	407	GLN

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Mol	Chain	Res	Type
1	M	423	ASN
1	M	434	ASN
1	N	86	ASN
1	N	311	ASN
1	N	347	GLN
1	N	404	GLN
1	N	434	ASN
1	N	447	HIS
1	O	19	ASN
1	O	86	ASN
1	O	157	GLN
1	O	329	HIS
1	O	404	GLN
1	O	477	HIS
1	P	18	ASN
1	P	86	ASN
1	P	101	ASN
1	P	113	HIS
1	P	157	GLN
1	P	162	ASN
1	P	170	GLN
1	P	266	ASN
1	P	280	ASN
1	P	385	GLN
1	P	434	ASN
1	Q	129	HIS
1	Q	185	ASN
1	Q	329	HIS
1	Q	380	HIS
1	Q	407	GLN
1	Q	430	HIS
1	Q	434	ASN
1	Q	447	HIS
1	R	86	ASN
1	R	157	GLN
1	R	224	HIS
1	R	233	HIS
1	R	280	ASN
1	R	347	GLN
1	R	380	HIS
1	R	393	ASN
1	R	423	ASN

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Mol	Chain	Res	Type
1	R	430	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	480/480 (100%)	-0.11	2 (0%)	88 86	26, 38, 59, 87	0
1	B	480/480 (100%)	0.01	8 (1%)	69 65	26, 41, 61, 97	0
1	C	480/480 (100%)	-0.17	2 (0%)	88 86	29, 38, 55, 97	0
1	D	480/480 (100%)	0.05	9 (1%)	66 62	29, 44, 60, 86	0
1	E	479/480 (99%)	-0.06	8 (1%)	69 65	26, 39, 64, 91	0
1	F	480/480 (100%)	0.13	9 (1%)	66 62	32, 46, 68, 94	0
1	G	479/480 (99%)	0.15	16 (3%)	49 45	29, 43, 71, 98	0
1	H	480/480 (100%)	0.15	16 (3%)	49 45	26, 44, 71, 87	0
1	I	480/480 (100%)	0.27	14 (2%)	53 50	32, 49, 72, 92	0
1	J	480/480 (100%)	0.25	10 (2%)	63 59	36, 48, 69, 93	0
1	K	480/480 (100%)	0.37	12 (2%)	58 54	28, 48, 65, 82	0
1	L	480/480 (100%)	0.35	24 (5%)	34 30	32, 50, 75, 90	0
1	M	480/480 (100%)	0.24	10 (2%)	63 59	34, 48, 70, 111	0
1	N	480/480 (100%)	0.42	21 (4%)	39 34	29, 52, 81, 105	0
1	O	480/480 (100%)	0.55	16 (3%)	49 45	39, 57, 79, 103	0
1	P	480/480 (100%)	0.89	39 (8%)	18 14	37, 64, 96, 112	0
1	Q	480/480 (100%)	0.29	14 (2%)	53 50	39, 51, 71, 100	0
1	R	480/480 (100%)	0.70	44 (9%)	14 12	30, 55, 79, 116	0
All	All	8638/8640 (99%)	0.25	274 (3%)	50 46	26, 47, 74, 116	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	480	CYS	5.2
1	R	326	ALA	5.1
1	L	324	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	R	328	ILE	4.4
1	L	325	ALA	4.3
1	R	140	VAL	3.9
1	K	279	ARG	3.8
1	R	279	ARG	3.7
1	H	280	ASN	3.7
1	N	480	CYS	3.7
1	P	328	ILE	3.7
1	I	155	THR	3.7
1	I	133	GLU	3.7
1	L	163	TYR	3.6
1	P	480	CYS	3.5
1	H	142	LEU	3.5
1	L	323	ARG	3.4
1	H	140	VAL	3.4
1	H	470	VAL	3.4
1	L	322	ARG	3.4
1	A	388	GLU	3.3
1	Q	473	GLY	3.3
1	I	139	GLU	3.3
1	R	50	GLY	3.3
1	R	327	ASN	3.2
1	H	144	ASP	3.2
1	O	244	ARG	3.2
1	O	280	ASN	3.2
1	Q	316	SER	3.1
1	R	65	GLY	3.1
1	L	64	VAL	3.1
1	O	70	ILE	3.1
1	B	339	CYS	3.1
1	B	480	CYS	3.0
1	L	480	CYS	3.0
1	P	132	LYS	3.0
1	R	60	VAL	3.0
1	R	55	LEU	3.0
1	L	131	ARG	3.0
1	P	185	ASN	3.0
1	F	328	ILE	3.0
1	P	470	VAL	3.0
1	R	16	ILE	3.0
1	R	73	PHE	3.0
1	G	328	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	392	ILE	3.0
1	O	479	GLU	3.0
1	G	144	ASP	3.0
1	B	472	THR	2.9
1	K	430	HIS	2.9
1	L	133	GLU	2.9
1	G	280	ASN	2.9
1	L	388	GLU	2.9
1	R	64	VAL	2.9
1	P	17	GLY	2.9
1	K	331	VAL	2.8
1	P	378	ASN	2.8
1	O	385	GLN	2.8
1	I	480	CYS	2.8
1	D	479	GLU	2.8
1	N	59	GLU	2.8
1	F	329	HIS	2.8
1	R	155	THR	2.8
1	B	479	GLU	2.8
1	R	385	GLN	2.8
1	P	475	THR	2.7
1	N	156	GLU	2.7
1	R	88	ILE	2.7
1	L	430	HIS	2.7
1	P	103	PHE	2.7
1	J	478	LEU	2.7
1	R	470	VAL	2.7
1	H	471	GLU	2.7
1	P	130	ILE	2.6
1	Q	103	PHE	2.6
1	K	133	GLU	2.6
1	Q	106	GLU	2.6
1	K	429	GLY	2.6
1	D	280	ASN	2.6
1	A	119	GLU	2.6
1	F	133	GLU	2.6
1	P	329	HIS	2.6
1	P	467	TYR	2.6
1	R	329	HIS	2.6
1	J	405	ASP	2.6
1	R	473	GLY	2.6
1	P	16	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	106	GLU	2.6
1	P	478	LEU	2.6
1	E	280	ASN	2.6
1	P	321	MET	2.5
1	M	478	LEU	2.5
1	J	385	GLN	2.5
1	M	480	CYS	2.5
1	L	279	ARG	2.5
1	L	479	GLU	2.5
1	Q	303	GLU	2.5
1	N	280	ASN	2.5
1	E	277	CYS	2.5
1	I	323	ARG	2.5
1	J	1	MET	2.5
1	F	332	GLY	2.5
1	G	145	GLY	2.5
1	F	313	ASP	2.5
1	H	479	GLU	2.5
1	K	407	GLN	2.5
1	R	74	THR	2.5
1	P	73	PHE	2.5
1	J	279	ARG	2.5
1	N	314	ALA	2.5
1	R	48	ALA	2.5
1	G	480	CYS	2.4
1	P	2	LEU	2.4
1	M	279	ARG	2.4
1	G	473	GLY	2.4
1	R	17	GLY	2.4
1	Q	405	ASP	2.4
1	L	107	TYR	2.4
1	Q	110	LEU	2.4
1	M	474	GLU	2.4
1	J	102	GLY	2.4
1	R	49	ASP	2.4
1	I	389	LEU	2.4
1	D	279	ARG	2.4
1	N	279	ARG	2.4
1	P	245	ARG	2.4
1	R	131	ARG	2.4
1	R	280	ASN	2.4
1	R	317	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	74	THR	2.4
1	R	386	SER	2.4
1	F	130	ILE	2.4
1	G	449	ASP	2.4
1	K	405	ASP	2.4
1	L	385	GLN	2.4
1	R	382	LEU	2.4
1	D	73	PHE	2.4
1	M	1	MET	2.4
1	Q	1	MET	2.4
1	R	43	PHE	2.4
1	P	140	VAL	2.4
1	E	139	GLU	2.4
1	N	71	GLU	2.4
1	O	404	GLN	2.3
1	R	99	ILE	2.3
1	H	400	GLU	2.3
1	J	381	GLU	2.3
1	O	71	GLU	2.3
1	Q	384	GLU	2.3
1	J	473	GLY	2.3
1	N	387	GLY	2.3
1	R	15	ARG	2.3
1	Q	385	GLN	2.3
1	B	133	GLU	2.3
1	B	325	ALA	2.3
1	G	472	THR	2.3
1	I	322	ARG	2.3
1	R	138	ARG	2.3
1	B	474	GLU	2.3
1	D	480	CYS	2.3
1	H	133	GLU	2.3
1	R	480	CYS	2.3
1	Q	107	TYR	2.3
1	O	245	ARG	2.3
1	J	472	THR	2.3
1	I	118	GLY	2.3
1	N	329	HIS	2.3
1	N	67	TRP	2.3
1	I	154	PHE	2.3
1	L	381	GLU	2.3
1	G	470	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	140	VAL	2.3
1	H	390	ARG	2.3
1	L	434	ASN	2.2
1	K	224	HIS	2.2
1	M	385	GLN	2.2
1	P	219	GLN	2.2
1	L	386	SER	2.2
1	N	134	LYS	2.2
1	O	110	LEU	2.2
1	P	110	LEU	2.2
1	O	216	TRP	2.2
1	R	67	TRP	2.2
1	F	119	GLU	2.2
1	I	137	PHE	2.2
1	R	137	PHE	2.2
1	P	112	VAL	2.2
1	P	279	ARG	2.2
1	P	327	ASN	2.2
1	G	163	TYR	2.2
1	G	329	HIS	2.2
1	L	129	HIS	2.2
1	M	118	GLY	2.2
1	N	17	GLY	2.2
1	R	142	LEU	2.2
1	R	35	ILE	2.2
1	H	156	GLU	2.2
1	P	133	GLU	2.2
1	Q	474	GLU	2.2
1	O	103	PHE	2.2
1	N	392	ILE	2.2
1	Q	324	SER	2.2
1	N	303	GLU	2.2
1	R	474	GLU	2.2
1	F	131	ARG	2.2
1	N	323	ARG	2.2
1	P	95	PHE	2.2
1	P	184	VAL	2.2
1	P	280	ASN	2.2
1	H	143	SER	2.2
1	G	166	ASP	2.2
1	R	156	GLU	2.2
1	P	111	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	224	HIS	2.1
1	P	385	GLN	2.1
1	B	473	GLY	2.1
1	O	290	GLY	2.1
1	P	3	LEU	2.1
1	R	153	THR	2.1
1	D	71	GLU	2.1
1	D	388	GLU	2.1
1	R	76	LYS	2.1
1	K	460	PHE	2.1
1	N	393	ASN	2.1
1	K	332	GLY	2.1
1	N	155	THR	2.1
1	C	476	ARG	2.1
1	G	479	GLU	2.1
1	K	244	ARG	2.1
1	N	131	ARG	2.1
1	P	165	SER	2.1
1	L	1	MET	2.1
1	E	470	VAL	2.1
1	H	75	ALA	2.1
1	R	108	ALA	2.1
1	P	31	LEU	2.1
1	P	148	THR	2.1
1	P	476	ARG	2.1
1	L	61	ASP	2.1
1	N	324	SER	2.1
1	E	140	VAL	2.1
1	N	470	VAL	2.1
1	R	51	GLY	2.1
1	H	472	THR	2.1
1	Q	388	GLU	2.1
1	O	328	ILE	2.1
1	F	215	ASP	2.1
1	P	69	ASP	2.1
1	R	150	VAL	2.0
1	I	244	ARG	2.0
1	K	314	ALA	2.0
1	O	279	ARG	2.0
1	P	326	ALA	2.0
1	M	280	ASN	2.0
1	P	246	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	471	GLU	2.0
1	G	400	GLU	2.0
1	L	164	GLU	2.0
1	R	63	LYS	2.0
1	I	324	SER	2.0
1	C	404	GLN	2.0
1	H	480	CYS	2.0
1	H	279	ARG	2.0
1	J	476	ARG	2.0
1	D	471	GLU	2.0
1	G	222	LEU	2.0
1	G	223	LYS	2.0
1	I	474	GLU	2.0
1	O	51	GLY	2.0
1	E	472	THR	2.0
1	N	320	ILE	2.0
1	O	56	THR	2.0
1	D	477	HIS	2.0
1	P	30	HIS	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.