



Full wwPDB X-ray Structure Validation Report

Nov 27, 2014 – 12:30 PM EST

PDB ID : 4V1C
Title : sirtuin 3
Authors : Wang, Y.; Hao, Q.
Deposited on : 2014-09-25
Resolution : 2.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

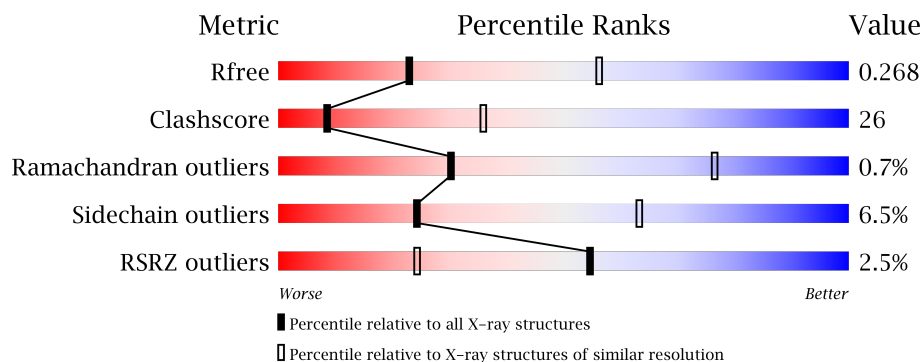
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24195
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 2.95 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}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	275	
2	E	275	
2	G	275	
2	K	275	
3	C	7	
3	D	7	
3	F	7	
3	H	7	
3	J	7	
3	L	7	
4	I	275	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	E	1395	-	X
6	GOL	E	1396	-	X
6	GOL	K	1395	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12026 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	1	1	0
			2112	1362	361	380	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	LYS	ARG	CONFLICT	UNP Q9NTG7

- Molecule 2 is a protein called NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	S	0	1	0
			2065	1335	353	368	9			
2	E	263	Total	C	N	O	S	1	1	0
			2059	1326	353	371	9			
2	G	252	Total	C	N	O	S	0	1	0
			1951	1259	335	349	8			
2	K	191	Total	C	N	O	S	1	1	0
			1474	945	260	265	4			

- Molecule 3 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			64	38	15	11			
3	D	7	Total	C	N	O	0	0	0
			64	38	15	11			
3	F	7	Total	C	N	O	0	0	0
			64	38	15	11			
3	H	7	Total	C	N	O	0	0	0
			64	38	15	11			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	7	Total	C	N	O	0	0	0
			64	38	15	11			
3	L	7	Total	C	N	O	0	0	0
			64	38	15	11			

- Molecule 4 is a protein called NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	251	Total	C	N	O	S	0	0	0
			1940	1251	336	344	9			

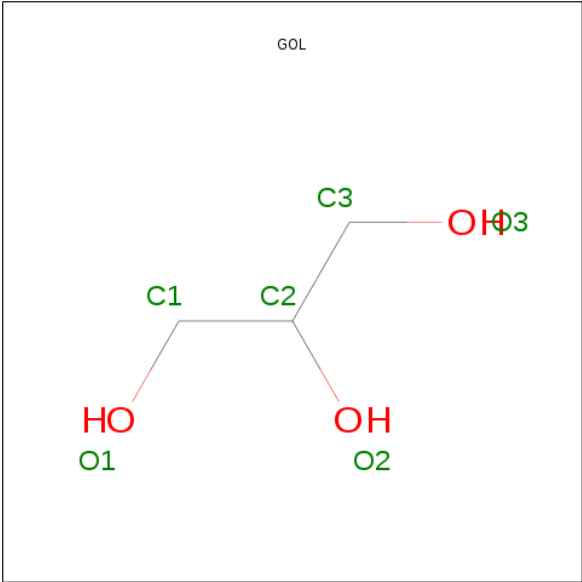
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	202	ALA	GLY	CONFLICT	UNP Q9NTG7

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Zn	0	0
			1	1		
5	G	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		

• Molecule 2: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain G:



• Molecule 2: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain K:



• Molecule 3: PEPTIDE

Chain C:



• Molecule 3: PEPTIDE

Chain D:



• Molecule 3: PEPTIDE

Chain F:



• Molecule 3: PEPTIDE

Chain H:





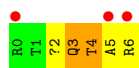
- Molecule 3: PEPTIDE

Chain J:



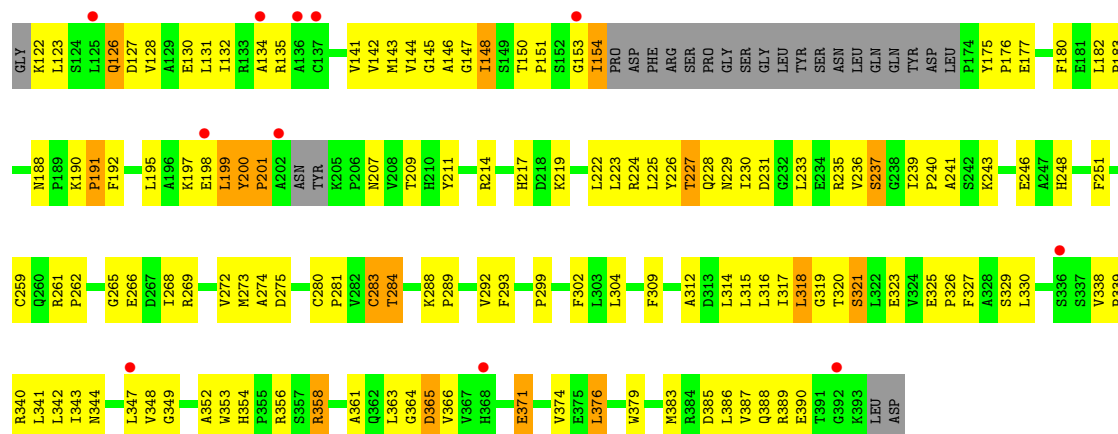
- Molecule 3: PEPTIDE

Chain L:



- Molecule 4: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	138.09Å 138.09Å 225.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.25 – 2.95 39.25 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.25-2.95) 94.2 (39.25-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.225 , 0.278 0.214 , 0.268	Depositor DCC
R_{free} test set	2318 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48352 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12026	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, BTK

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.77	1/2170 (0.0%)	0.73	1/2956 (0.0%)
2	B	0.63	0/2123	0.72	2/2894 (0.1%)
2	E	0.62	0/2112	0.68	0/2876
2	G	0.57	1/2003 (0.0%)	0.67	1/2725 (0.0%)
2	K	0.49	0/1507	0.67	1/2049 (0.0%)
3	C	0.40	0/48	0.58	0/61
3	D	0.37	0/48	0.63	0/61
3	F	0.36	0/48	0.61	0/61
3	H	0.34	0/48	0.62	0/61
3	J	0.34	0/48	0.66	0/61
3	L	0.30	0/48	0.60	0/61
4	I	0.64	1/1986 (0.1%)	0.71	3/2705 (0.1%)
All	All	0.63	3/12189 (0.0%)	0.70	8/16571 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	283	CYS	CB-SG	-9.15	1.66	1.82
2	G	256	CYS	CB-SG	8.51	1.96	1.82
1	A	137	CYS	CB-SG	-6.57	1.71	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	274	ALA	N-CA-C	9.50	136.65	111.00
4	I	201	PRO	N-CA-CB	6.19	110.73	103.30
2	K	244	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	201	PRO	CA-C-N	5.99	128.19	116.20
2	G	281	PRO	N-CA-CB	5.81	110.27	103.30
4	I	283	CYS	N-CA-C	5.39	125.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	LEU	CB-CG-CD1	-5.36	101.90	111.00
2	B	225	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2112	0	2123	98	0
2	B	2065	0	2073	81	0
2	E	2059	0	2068	75	0
2	G	1951	0	1961	132	0
2	K	1474	0	1498	87	0
3	C	64	0	71	5	0
3	D	64	0	71	4	0
3	F	64	0	71	10	0
3	H	64	0	71	7	0
3	J	64	0	71	13	0
3	L	64	0	72	9	0
4	I	1940	0	1947	142	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	2	0
5	I	1	0	0	0	0
6	B	6	0	8	4	0
6	E	12	0	16	0	0
6	G	6	0	8	0	0
6	I	6	0	8	1	0
6	K	6	0	8	2	0
All	All	12026	0	12145	625	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 26.

All (625) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:283:CYS:SG	5:G:1395:ZN:ZN	1.03	1.48
2:G:280:CYS:SG	2:G:283:CYS:HB2	1.60	1.40
2:K:347:LEU:HD23	2:K:347:LEU:C	1.49	1.22
2:B:159:SER:CB	2:B:160:PRO:HA	1.65	1.22
2:G:280:CYS:SG	2:G:283:CYS:CB	2.36	1.12
3:J:0:ARG:HG2	3:J:0:ARG:HH11	1.04	1.11
4:I:199:LEU:N	4:I:199:LEU:HD12	1.66	1.10
2:B:159:SER:CB	2:B:160:PRO:CA	2.30	1.08
4:I:207:ASN:OD1	4:I:209:THR:HG22	1.56	1.05
1:A:320:THR:HG22	1:A:322:LEU:H	1.16	1.03
4:I:180:PHE:CE2	3:J:2:BTK:HAF	1.93	1.03
2:K:347:LEU:HD21	2:K:352:ALA:HB2	1.39	1.03
2:G:256:CYS:SG	2:G:280:CYS:HB2	1.99	1.01
2:G:188:ASN:OD1	2:G:191:PRO:HD3	1.60	0.99
2:G:244:LEU:H	2:G:244:LEU:HD12	1.28	0.99
2:K:347:LEU:CD2	2:K:347:LEU:C	2.30	0.98
2:K:230:ILE:HD12	2:K:251:PHE:CZ	1.99	0.97
2:K:347:LEU:O	2:K:347:LEU:HD23	1.63	0.96
2:G:280:CYS:HB3	2:G:283:CYS:O	1.66	0.96
1:A:190:LYS:NZ	1:A:275:ASP:OD1	1.99	0.96
4:I:283:CYS:O	4:I:284:THR:HG23	1.65	0.95
2:G:280:CYS:CB	2:G:283:CYS:HB2	1.96	0.95
4:I:199:LEU:CD1	4:I:199:LEU:N	2.29	0.95
2:G:148:ILE:HB	2:G:209:THR:HG21	1.46	0.94
2:B:320:THR:HG22	2:B:322:LEU:H	1.34	0.91
1:A:148:ILE:CG2	1:A:209:THR:HG21	2.02	0.90
1:A:157:PHE:O	1:A:176:PRO:HB3	1.72	0.90
2:G:283:CYS:HG	5:G:1395:ZN:ZN	0.65	0.89
2:G:256:CYS:SG	2:G:283:CYS:HB2	2.12	0.89
2:G:256:CYS:SG	2:G:283:CYS:CB	2.62	0.87
3:J:0:ARG:NH1	3:J:0:ARG:HG2	1.82	0.87
4:I:228:GLN:HG3	4:I:248:HIS:CE1	2.10	0.86
2:B:387:VAL:O	2:B:391:THR:OG1	1.92	0.85
2:E:259:CYS:SG	2:E:261:ARG:HG3	2.16	0.85
2:G:179:ILE:HD11	2:G:192:PHE:HA	1.61	0.82
2:G:175:TYR:HB2	2:G:176:PRO:HD2	1.60	0.82
4:I:146:ALA:O	4:I:150:THR:HG23	1.80	0.81
2:B:253:SER:HB2	2:B:290:ASP:OD2	1.79	0.81
2:E:387:VAL:O	2:E:391:THR:HB	1.80	0.81
2:G:244:LEU:HD12	2:G:244:LEU:N	1.92	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:325:GLU:HG3	4:I:326:PRO:HA	1.61	0.81
2:G:280:CYS:HG	2:G:283:CYS:HB2	1.43	0.81
1:A:148:ILE:HG22	1:A:209:THR:HG21	1.64	0.80
4:I:199:LEU:CD1	4:I:199:LEU:H	1.93	0.80
4:I:321:SER:O	4:I:348:VAL:HG11	1.80	0.80
2:B:159:SER:CB	2:B:160:PRO:O	2.30	0.80
2:E:248:HIS:ND1	3:F:2:BTK:HAJ	1.97	0.80
4:I:268:ILE:O	4:I:272:VAL:HG23	1.81	0.80
4:I:283:CYS:O	4:I:284:THR:CG2	2.29	0.80
2:G:154:ILE:HB	2:G:155:PRO:HD3	1.64	0.79
4:I:198:GLU:HB2	4:I:199:LEU:HD12	1.64	0.79
4:I:175:TYR:HB2	4:I:176:PRO:CD	2.13	0.78
2:K:347:LEU:HD23	2:K:348:VAL:N	1.96	0.78
2:G:256:CYS:SG	2:G:280:CYS:CB	2.71	0.78
2:G:150:THR:HB	2:G:151:PRO:HD3	1.65	0.78
4:I:361:ALA:HB1	4:I:363:LEU:CD1	2.13	0.78
2:G:184:PHE:O	2:G:184:PHE:HD1	1.66	0.78
2:G:280:CYS:CB	2:G:283:CYS:O	2.31	0.78
2:K:142:VAL:HG22	2:K:316:LEU:HB2	1.66	0.78
2:B:264:PRO:HG3	2:B:267:ASP:OD2	1.84	0.77
2:K:230:ILE:HD12	2:K:251:PHE:CE1	2.18	0.77
4:I:371:GLU:HA	4:I:374:VAL:HG22	1.66	0.77
2:B:353:TRP:HD1	2:B:354:HIS:ND1	1.82	0.77
1:A:160:PRO:HD3	1:A:167:ASN:H	1.51	0.75
1:A:347:LEU:HD12	1:A:352:ALA:HB2	1.68	0.75
3:L:5:ALA:O	3:L:6:ARG:HB2	1.86	0.75
2:G:189:PRO:HB2	2:G:193:PHE:HE2	1.50	0.75
2:G:175:TYR:HB2	2:G:176:PRO:CD	2.17	0.75
2:K:347:LEU:CD2	2:K:347:LEU:O	2.30	0.74
2:B:265:GLY:HA2	2:B:268:ILE:HG12	1.67	0.74
2:K:363:LEU:H	2:K:363:LEU:HD22	1.53	0.74
1:A:159:SER:HB3	1:A:160:PRO:HA	1.69	0.73
2:B:230:ILE:O	2:B:230:ILE:HG13	1.88	0.73
4:I:259:CYS:SG	4:I:261:ARG:HD2	2.29	0.73
2:E:176:PRO:HG2	2:E:177:GLU:OE2	1.89	0.73
1:A:154:ILE:H	1:A:154:ILE:HD12	1.54	0.73
4:I:143:MET:HG3	4:I:315:LEU:HD11	1.71	0.73
2:G:292:VAL:HG12	3:H:2:BTK:HD3	1.71	0.72
2:B:124:SER:O	2:B:127:ASP:HB2	1.89	0.72
2:G:178:ALA:HA	2:G:181:GLU:HG3	1.71	0.72
2:E:151:PRO:HG2	2:E:207:ASN:ND2	2.05	0.71
4:I:180:PHE:CD2	3:J:2:BTK:HAF	2.24	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:280:CYS:C	2:G:283:CYS:O	2.29	0.71
1:A:266:GLU:H	1:A:266:GLU:CD	1.93	0.71
2:E:227:THR:OG1	2:E:229:ASN:HB2	1.91	0.71
2:E:156:ASP:C	2:E:156:ASP:OD1	2.29	0.70
2:B:258:VAL:HG21	2:B:285:GLY:HA3	1.74	0.70
2:E:250:THR:O	2:E:291:ILE:CD1	2.40	0.70
2:K:210:HIS:CE1	2:K:233:LEU:HB3	2.27	0.70
2:E:141:VAL:O	2:E:315:LEU:HD12	1.92	0.69
4:I:198:GLU:HB2	4:I:199:LEU:CD1	2.22	0.69
2:E:125:LEU:HD11	2:E:373:LEU:HB2	1.74	0.69
2:K:153:GLY:O	2:K:154:ILE:HG13	1.93	0.69
4:I:321:SER:C	4:I:348:VAL:HG11	2.13	0.69
2:K:363:LEU:HD22	2:K:363:LEU:N	2.07	0.69
2:B:353:TRP:CD1	2:B:354:HIS:ND1	2.61	0.69
2:G:179:ILE:HD11	2:G:192:PHE:CA	2.22	0.69
2:B:256:CYS:SG	2:B:258:VAL:HG23	2.33	0.68
4:I:197:LYS:HE3	4:I:273:MET:O	1.93	0.68
4:I:321:SER:O	4:I:348:VAL:CG1	2.40	0.68
2:K:341:LEU:HD13	2:K:360:VAL:HG12	1.75	0.68
1:A:264:PRO:HB2	1:A:266:GLU:OE1	1.93	0.68
4:I:180:PHE:CZ	3:J:2:BTK:HAF	2.28	0.68
2:G:263:PHE:CD1	2:G:263:PHE:N	2.62	0.68
4:I:175:TYR:HB2	4:I:176:PRO:HD2	1.75	0.68
4:I:340:ARG:NH1	4:I:356:ARG:HD2	2.08	0.68
2:B:156:ASP:OD1	2:B:156:ASP:C	2.29	0.67
2:K:351:LEU:HD22	2:K:351:LEU:N	2.08	0.67
1:A:320:THR:HG22	1:A:322:LEU:N	2.01	0.67
2:E:208:VAL:HG23	2:E:383:MET:CE	2.24	0.67
2:G:385:ASP:O	2:G:389:ARG:HG3	1.95	0.67
1:A:180:PHE:CD2	3:C:2:BTK:HAJA	2.29	0.67
2:G:294:PHE:CE1	3:H:4:THR:HG22	2.29	0.67
2:G:342:LEU:CD2	2:G:344:ASN:HB2	2.24	0.67
2:B:263:PHE:HB3	2:B:264:PRO:HD2	1.77	0.67
4:I:141:VAL:HG22	4:I:223:LEU:HD23	1.76	0.66
4:I:200:TYR:CE2	4:I:269:ARG:HG3	2.30	0.66
2:B:156:ASP:OD1	2:B:158:ARG:N	2.29	0.66
2:G:280:CYS:HB3	2:G:283:CYS:C	2.15	0.66
2:G:256:CYS:HG	2:G:283:CYS:CB	2.07	0.66
2:G:342:LEU:HD21	2:G:344:ASN:HB2	1.78	0.66
4:I:347:LEU:HD12	4:I:348:VAL:H	1.59	0.66
2:B:353:TRP:HD1	2:B:354:HIS:CE1	2.13	0.66
2:B:353:TRP:CD1	2:B:354:HIS:CE1	2.84	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:150:THR:OG1	4:I:151:PRO:HD3	1.96	0.66
2:G:280:CYS:SG	2:G:283:CYS:CA	2.82	0.66
2:K:363:LEU:CD2	2:K:363:LEU:H	2.09	0.66
1:A:159:SER:CB	1:A:160:PRO:HA	2.25	0.66
1:A:160:PRO:HD3	1:A:167:ASN:HB2	1.77	0.66
4:I:353:TRP:HA	4:I:353:TRP:CE3	2.30	0.66
2:K:294:PHE:HE1	3:L:4:THR:N	1.94	0.66
2:B:140:VAL:HG22	2:B:314:LEU:HD23	1.79	0.65
2:G:282:VAL:N	2:G:283:CYS:O	2.30	0.65
1:A:185:PHE:O	1:A:189:PRO:HG3	1.95	0.65
1:A:156:ASP:O	1:A:157:PHE:HB2	1.95	0.65
2:G:280:CYS:N	2:G:285:GLY:O	2.29	0.65
2:K:344:ASN:O	2:K:363:LEU:HA	1.97	0.65
4:I:227:THR:OG1	4:I:229:ASN:HB2	1.96	0.64
4:I:353:TRP:HA	4:I:353:TRP:HE3	1.62	0.64
2:G:228:GLN:HG2	2:G:248:HIS:NE2	2.13	0.64
1:A:323:GLU:HG3	1:A:324:VAL:HG23	1.79	0.64
1:A:259:CYS:HB3	1:A:283:CYS:SG	2.39	0.63
2:B:159:SER:CB	2:B:160:PRO:C	2.66	0.63
2:G:280:CYS:SG	2:G:283:CYS:N	2.71	0.63
4:I:222:LEU:O	4:I:243:LYS:HE3	1.97	0.63
1:A:268:ILE:HD11	1:A:289:PRO:HG3	1.79	0.63
4:I:176:PRO:HG2	4:I:177:GLU:H	1.63	0.63
1:A:309:PHE:CE2	1:A:330:LEU:HB3	2.34	0.63
4:I:228:GLN:HB2	4:I:327:PHE:CE2	2.33	0.62
4:I:195:LEU:O	4:I:199:LEU:HD13	1.99	0.62
2:K:356:ARG:N	2:K:359:ASP:OD2	2.32	0.62
1:A:139:ARG:HB2	1:A:313:ASP:OD1	1.99	0.62
1:A:339:PRO:HA	1:A:358:ARG:O	1.98	0.62
4:I:321:SER:HB2	4:I:323:GLU:OE1	2.00	0.62
2:B:158:ARG:NH2	2:B:177:GLU:OE2	2.21	0.62
2:K:230:ILE:HD12	2:K:251:PHE:HZ	1.63	0.61
2:G:280:CYS:HG	2:G:283:CYS:CB	2.05	0.61
2:E:209:THR:HG23	2:E:370:VAL:HG21	1.82	0.61
2:E:180:PHE:CE2	3:F:2:BTK:HAF	2.36	0.61
2:G:347:LEU:O	2:G:348:VAL:HG13	2.00	0.61
2:G:256:CYS:O	2:G:286:VAL:O	2.18	0.61
4:I:224:ARG:HG2	4:I:226:TYR:CE1	2.35	0.61
2:K:370:VAL:O	2:K:374:VAL:HG23	2.00	0.61
4:I:122:LYS:HG3	4:I:123:LEU:N	2.16	0.61
4:I:339:PRO:HA	4:I:358:ARG:HB2	1.81	0.61
1:A:200:TYR:C	1:A:201:PRO:O	2.39	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:354:HIS:N	2:E:355:PRO:HD3	2.15	0.60
4:I:315:LEU:HD12	4:I:316:LEU:N	2.17	0.60
2:K:347:LEU:CD2	2:K:352:ALA:HB2	2.24	0.60
2:G:244:LEU:H	2:G:244:LEU:CD1	2.09	0.60
2:E:250:THR:O	2:E:291:ILE:HD13	2.02	0.60
2:E:353:TRP:C	2:E:355:PRO:HD3	2.21	0.60
2:G:256:CYS:SG	2:G:283:CYS:HB3	2.42	0.60
2:K:215:LEU:HD23	2:K:379:TRP:HE3	1.67	0.60
4:I:141:VAL:CG2	4:I:312:ALA:HB2	2.31	0.60
2:B:190:LYS:HB2	2:B:191:PRO:HD3	1.84	0.60
2:G:189:PRO:C	2:G:191:PRO:HD2	2.23	0.60
2:G:263:PHE:HD1	2:G:263:PHE:N	2.00	0.60
2:K:209:THR:HG22	2:K:370:VAL:HG21	1.83	0.60
2:E:298:LEU:HB3	2:E:299:PRO:HD2	1.83	0.59
2:E:314:LEU:HD13	2:E:339:PRO:HG2	1.85	0.59
3:J:0:ARG:CG	3:J:0:ARG:HH11	1.95	0.59
2:E:145:GLY:HA3	2:E:320:THR:HB	1.85	0.59
2:G:189:PRO:HB2	2:G:193:PHE:CE2	2.35	0.59
1:A:304:LEU:HD21	2:B:303:LEU:HD12	1.85	0.59
4:I:144:VAL:HB	4:I:148:ILE:HD13	1.84	0.59
2:E:142:VAL:HG21	2:E:213:LEU:HD22	1.84	0.59
4:I:292:VAL:HG21	4:I:299:PRO:HD3	1.84	0.59
4:I:371:GLU:O	4:I:374:VAL:HG22	2.03	0.59
2:K:292:VAL:CG1	3:L:2:BTK:HD3	2.33	0.58
2:B:298:LEU:HB3	2:B:299:PRO:HD2	1.85	0.58
2:G:174:PRO:HB2	2:G:175:TYR:CD1	2.38	0.58
1:A:385:ASP:OD2	4:I:135:ARG:NH1	2.35	0.58
2:G:182:LEU:N	2:G:183:PRO:HD2	2.19	0.58
4:I:343:ILE:HG22	4:I:366:VAL:HG23	1.84	0.58
2:B:320:THR:HG23	6:B:1396:GOL:O3	2.04	0.58
2:G:228:GLN:HG2	2:G:248:HIS:CD2	2.39	0.58
2:K:210:HIS:CE1	2:K:233:LEU:CB	2.87	0.58
2:K:230:ILE:CD1	2:K:251:PHE:CZ	2.82	0.58
2:B:258:VAL:CG2	2:B:285:GLY:HA3	2.33	0.58
4:I:386:LEU:HD12	4:I:390:GLU:HG2	1.86	0.58
2:E:150:THR:N	2:E:151:PRO:HD2	2.19	0.57
2:G:184:PHE:O	2:G:184:PHE:CD1	2.54	0.57
2:B:177:GLU:N	2:B:177:GLU:OE1	2.29	0.57
4:I:180:PHE:CE2	3:J:2:BTK:CAF	2.81	0.57
2:K:148:ILE:HD12	2:K:210:HIS:NE2	2.19	0.57
2:K:228:GLN:OE1	6:K:1395:GOL:H2	2.04	0.57
1:A:147:GLY:HA3	1:A:319:GLY:HA3	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:VAL:HG21	1:A:312:ALA:HB2	1.85	0.57
4:I:338:VAL:HG12	4:I:339:PRO:O	2.05	0.57
4:I:198:GLU:C	4:I:199:LEU:HD12	2.22	0.57
1:A:147:GLY:HA3	1:A:319:GLY:CA	2.34	0.56
2:G:263:PHE:HB3	2:G:264:PRO:CD	2.34	0.56
4:I:145:GLY:HA3	4:I:320:THR:HB	1.87	0.56
2:K:123:LEU:O	2:K:360:VAL:HG22	2.05	0.56
4:I:344:ASN:O	4:I:363:LEU:HA	2.04	0.56
3:L:3:GLN:HG2	3:L:4:THR:O	2.06	0.56
1:A:268:ILE:O	1:A:272:VAL:HG23	2.05	0.56
2:G:184:PHE:C	2:G:184:PHE:CD1	2.77	0.56
2:G:179:ILE:HD11	2:G:192:PHE:N	2.21	0.56
1:A:321:SER:O	1:A:348:VAL:CG2	2.54	0.56
2:E:168:LEU:HD13	2:E:173:LEU:HB2	1.87	0.56
1:A:148:ILE:HG21	1:A:209:THR:HG21	1.84	0.56
2:B:262:PRO:C	2:B:263:PHE:CD1	2.79	0.56
2:B:298:LEU:N	2:B:298:LEU:HD23	2.21	0.56
4:I:283:CYS:C	4:I:284:THR:CG2	2.71	0.56
2:K:387:VAL:O	2:K:391:THR:HG23	2.06	0.56
2:E:341:LEU:HD12	2:E:342:LEU:N	2.20	0.55
4:I:176:PRO:HG2	4:I:177:GLU:N	2.20	0.55
2:G:175:TYR:H	2:G:175:TYR:HD1	1.53	0.55
2:G:234:GLU:CD	2:G:234:GLU:H	2.09	0.55
2:G:353:TRP:HD1	2:G:354:HIS:CD2	2.25	0.55
1:A:159:SER:HB3	1:A:160:PRO:CA	2.37	0.55
2:B:370:VAL:O	2:B:374:VAL:HG23	2.05	0.55
4:I:147:GLY:N	4:I:319:GLY:O	2.39	0.55
2:K:363:LEU:CD2	2:K:363:LEU:N	2.65	0.55
1:A:177:GLU:HB2	1:A:294:PHE:CE2	2.42	0.55
2:B:264:PRO:CG	2:B:267:ASP:OD2	2.54	0.55
2:E:327:PHE:O	2:E:330:LEU:HB2	2.07	0.55
1:A:259:CYS:SG	1:A:261:ARG:HG3	2.47	0.55
2:E:309:PHE:CZ	2:E:330:LEU:HD13	2.42	0.55
1:A:261:ARG:HH11	1:A:261:ARG:HG2	1.70	0.54
2:B:151:PRO:HG2	2:B:207:ASN:ND2	2.23	0.54
4:I:175:TYR:HB2	4:I:176:PRO:HD3	1.88	0.54
2:B:268:ILE:O	2:B:272:VAL:HG23	2.07	0.54
2:B:321:SER:HB2	2:B:323:GLU:HG3	1.88	0.54
1:A:353:TRP:CH2	3:C:6:ARG:HB2	2.42	0.54
4:I:153:GLY:O	4:I:154:ILE:HG13	2.07	0.54
2:G:183:PRO:HG2	2:G:184:PHE:H	1.72	0.54
2:G:256:CYS:O	2:G:257:THR:CB	2.55	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:323:GLU:HA	3:L:5:ALA:HB3	1.89	0.54
1:A:224:ARG:HG2	1:A:226:TYR:CE1	2.42	0.54
4:I:175:TYR:CB	4:I:176:PRO:CD	2.82	0.54
1:A:200:TYR:CB	1:A:201:PRO:HD3	2.38	0.54
3:D:1:THR:O	3:D:3:GLN:HG2	2.08	0.54
2:K:143:MET:HB3	2:K:327:PHE:CE1	2.43	0.54
2:K:341:LEU:HD13	2:K:360:VAL:CG1	2.38	0.54
2:K:366:VAL:CG2	2:K:367:VAL:N	2.70	0.54
1:A:154:ILE:HD12	1:A:154:ILE:N	2.22	0.54
4:I:150:THR:N	4:I:151:PRO:CD	2.71	0.54
4:I:198:GLU:CB	4:I:199:LEU:HD12	2.36	0.53
2:K:318:LEU:CD2	2:K:343:ILE:HB	2.37	0.53
2:B:385:ASP:OD2	2:E:135:ARG:NH1	2.41	0.53
2:E:174:PRO:HB2	2:E:175:TYR:CD1	2.43	0.53
2:G:228:GLN:HG3	2:G:327:PHE:CD2	2.43	0.53
4:I:135:ARG:NH2	4:I:219:LYS:O	2.41	0.53
1:A:176:PRO:HG2	1:A:177:GLU:OE2	2.08	0.53
2:B:228:GLN:HB3	6:B:1396:GOL:H11	1.90	0.53
2:E:125:LEU:HD22	2:E:362:GLN:OE1	2.08	0.53
2:K:341:LEU:CD1	2:K:360:VAL:HG12	2.39	0.53
2:E:279:ARG:HD2	2:E:284:THR:O	2.08	0.53
4:I:141:VAL:HG23	4:I:312:ALA:HB2	1.89	0.53
1:A:370:VAL:O	1:A:374:VAL:HG23	2.08	0.53
2:K:143:MET:HA	2:K:226:TYR:O	2.08	0.53
1:A:133:ARG:NH1	1:A:377:LEU:O	2.42	0.53
2:K:300:GLN:OE1	2:K:300:GLN:HA	2.08	0.53
2:K:309:PHE:CZ	2:K:330:LEU:HB3	2.43	0.53
1:A:309:PHE:CZ	1:A:330:LEU:HD13	2.43	0.53
4:I:348:VAL:HG12	4:I:349:GLY:N	2.22	0.53
2:K:150:THR:OG1	2:K:151:PRO:HD3	2.09	0.53
2:K:215:LEU:HD23	2:K:379:TRP:CE3	2.44	0.53
2:E:125:LEU:HG	2:E:376:LEU:HD12	1.90	0.53
4:I:141:VAL:CG2	4:I:223:LEU:HD23	2.39	0.52
3:J:0:ARG:HD3	3:J:0:ARG:C	2.29	0.52
2:B:392:GLY:C	2:B:394:LEU:H	2.13	0.52
2:G:317:ILE:HD13	2:G:317:ILE:O	2.09	0.52
2:B:215:LEU:HD11	2:B:219:LYS:HE2	1.90	0.52
2:E:367:VAL:O	2:E:371:GLU:HG3	2.09	0.52
2:G:292:VAL:O	3:H:2:BTK:NZ	2.42	0.52
4:I:134:ALA:O	4:I:135:ARG:HB2	2.09	0.52
4:I:176:PRO:CG	4:I:177:GLU:H	2.21	0.52
4:I:340:ARG:HH11	4:I:356:ARG:HH11	1.56	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:361:ALA:HB1	4:I:363:LEU:HD11	1.88	0.52
4:I:383:MET:O	4:I:387:VAL:HG23	2.09	0.52
2:E:175:TYR:HB2	2:E:176:PRO:HD2	1.92	0.52
4:I:340:ARG:NH1	4:I:356:ARG:HH11	2.08	0.52
4:I:176:PRO:CG	4:I:177:GLU:N	2.72	0.52
2:G:230:ILE:HG21	2:G:291:ILE:HD12	1.92	0.52
2:G:342:LEU:HD22	2:G:343:ILE:N	2.24	0.52
4:I:239:ILE:HG23	4:I:240:PRO:HD2	1.92	0.52
2:G:178:ALA:HB1	2:G:184:PHE:HD2	1.75	0.52
2:G:184:PHE:C	2:G:184:PHE:HD1	2.12	0.51
4:I:143:MET:O	4:I:317:ILE:HA	2.10	0.51
4:I:147:GLY:O	4:I:151:PRO:CD	2.58	0.51
4:I:228:GLN:O	4:I:228:GLN:HG2	2.10	0.51
1:A:151:PRO:HB2	1:A:207:ASN:ND2	2.25	0.51
2:K:146:ALA:O	2:K:150:THR:HG23	2.10	0.51
4:I:343:ILE:HD12	4:I:343:ILE:N	2.25	0.51
2:B:200:TYR:HE2	2:B:272:VAL:HG11	1.75	0.51
4:I:371:GLU:CA	4:I:374:VAL:HG22	2.39	0.51
2:G:294:PHE:HA	3:H:2:BTK:HB2	1.93	0.51
4:I:230:ILE:HD13	3:J:2:BTK:HAAA	1.93	0.51
4:I:361:ALA:HB1	4:I:363:LEU:HD12	1.93	0.51
1:A:258:VAL:HB	1:A:283:CYS:SG	2.50	0.51
2:G:316:LEU:HD13	2:G:341:LEU:HD23	1.92	0.51
4:I:199:LEU:HD13	4:I:199:LEU:H	1.72	0.51
1:A:180:PHE:CE2	3:C:2:BTK:HAAA	2.45	0.50
2:G:342:LEU:CD2	2:G:343:ILE:N	2.74	0.50
2:K:150:THR:HG22	2:K:154:ILE:O	2.11	0.50
1:A:298:LEU:HB3	1:A:299:PRO:HD2	1.93	0.50
2:G:179:ILE:HD11	2:G:191:PRO:C	2.31	0.50
2:G:268:ILE:O	2:G:268:ILE:HG13	2.12	0.50
2:K:124:SER:HB3	2:K:127:ASP:CG	2.32	0.50
1:A:200:TYR:O	1:A:201:PRO:O	2.30	0.50
2:G:301:ARG:NH1	2:G:304:LEU:HD11	2.27	0.50
2:B:140:VAL:CG2	2:B:314:LEU:HD23	2.40	0.50
2:G:177:GLU:O	2:G:181:GLU:HG2	2.11	0.50
4:I:251:PHE:O	4:I:265:GLY:HA3	2.11	0.50
4:I:348:VAL:CG1	4:I:349:GLY:N	2.74	0.50
2:K:226:TYR:CE1	2:K:245:VAL:HG11	2.47	0.50
2:E:346:ASP:HA	2:E:363:LEU:HD13	1.94	0.50
2:G:279:ARG:HA	2:G:286:VAL:HA	1.94	0.50
2:B:198:GLU:OE2	2:B:203:ASN:ND2	2.44	0.50
2:E:248:HIS:ND1	3:F:2:BTK:CAJ	2.73	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:256:CYS:SG	2:G:280:CYS:SG	3.09	0.50
1:A:230:ILE:O	1:A:230:ILE:HG13	2.12	0.50
2:B:230:ILE:HG23	3:D:2:BTK:HAAB	1.93	0.50
2:B:354:HIS:N	2:B:355:PRO:HD3	2.27	0.50
2:G:135:ARG:NH1	2:G:221:LEU:HD21	2.26	0.50
2:G:256:CYS:HA	2:G:287:VAL:HA	1.93	0.50
4:I:175:TYR:CB	4:I:176:PRO:HD2	2.42	0.50
2:B:392:GLY:O	2:B:394:LEU:N	2.45	0.49
4:I:217:HIS:ND1	4:I:243:LYS:HD2	2.27	0.49
2:G:280:CYS:O	2:G:283:CYS:O	2.29	0.49
4:I:175:TYR:HD2	4:I:176:PRO:HD2	1.77	0.49
1:A:170:GLN:HB3	1:A:171:TYR:CD1	2.47	0.49
2:G:344:ASN:O	2:G:363:LEU:HA	2.12	0.49
2:K:231:ASP:OD1	2:K:231:ASP:O	2.29	0.49
1:A:166:SER:O	1:A:169:GLN:N	2.42	0.49
1:A:317:ILE:N	1:A:317:ILE:HD12	2.28	0.49
2:G:176:PRO:C	2:G:178:ALA:H	2.14	0.49
2:B:224:ARG:HG2	2:B:226:TYR:CE1	2.47	0.49
4:I:222:LEU:HD12	4:I:223:LEU:H	1.78	0.49
2:E:346:ASP:OD1	2:E:346:ASP:N	2.46	0.49
3:F:0:ARG:HD3	3:F:1:THR:N	2.28	0.49
4:I:288:LYS:HD2	4:I:293:PHE:CZ	2.48	0.49
1:A:171:TYR:CD1	1:A:171:TYR:N	2.80	0.49
2:G:280:CYS:HB3	2:G:283:CYS:HB2	1.90	0.49
2:E:139:ARG:HB3	2:E:223:LEU:HD22	1.95	0.49
2:E:259:CYS:O	2:E:260:GLN:HB2	2.13	0.49
4:I:385:ASP:O	4:I:388:GLN:HB3	2.13	0.49
2:K:289:PRO:O	2:K:291:ILE:N	2.46	0.49
2:K:292:VAL:HG12	3:L:2:BTK:HD3	1.94	0.49
2:K:230:ILE:CD1	2:K:251:PHE:HZ	2.25	0.48
2:B:126:GLN:HA	2:B:376:LEU:HD13	1.94	0.48
2:E:180:PHE:CE2	3:F:2:BTK:CAF	2.96	0.48
2:G:178:ALA:HB1	2:G:184:PHE:CD2	2.47	0.48
4:I:175:TYR:CD2	4:I:176:PRO:HD2	2.48	0.48
1:A:321:SER:OG	1:A:323:GLU:HG2	2.14	0.48
2:B:346:ASP:N	2:B:346:ASP:OD1	2.46	0.48
4:I:353:TRP:CA	4:I:353:TRP:CE3	2.97	0.48
3:L:5:ALA:O	3:L:6:ARG:CB	2.60	0.48
4:I:237:SER:OG	4:I:239:ILE:HD12	2.14	0.48
4:I:261:ARG:HA	4:I:262:PRO:HD3	1.61	0.48
3:J:5:ALA:O	3:J:6:ARG:HB2	2.13	0.48
1:A:154:ILE:H	1:A:154:ILE:CD1	2.24	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:394:LEU:O	2:E:394:LEU:HG	2.13	0.48
4:I:341:LEU:HD21	4:I:343:ILE:HD11	1.95	0.48
2:E:248:HIS:CG	3:F:2:BTK:HAJ	2.48	0.48
2:G:282:VAL:CA	2:G:283:CYS:C	2.81	0.48
2:G:193:PHE:HA	2:G:196:ALA:HB3	1.96	0.48
4:I:142:VAL:HG12	4:I:144:VAL:HG13	1.95	0.48
2:K:291:ILE:HG22	2:K:292:VAL:N	2.28	0.48
2:E:190:LYS:HD3	2:E:190:LYS:HA	1.68	0.47
2:E:211:TYR:HB3	2:E:386:LEU:HD23	1.95	0.47
4:I:182:LEU:HB2	4:I:183:PRO:HD3	1.95	0.47
2:K:298:LEU:HD12	2:K:298:LEU:H	1.79	0.47
2:G:240:PRO:O	2:G:243:LYS:HB2	2.14	0.47
2:B:321:SER:CB	2:B:323:GLU:HG3	2.43	0.47
2:G:154:ILE:CB	2:G:155:PRO:HD3	2.39	0.47
4:I:190:LYS:N	4:I:191:PRO:CD	2.77	0.47
2:B:381:GLU:O	2:B:384:ARG:HB3	2.15	0.47
2:E:168:LEU:O	2:E:172:ASP:N	2.47	0.47
2:E:344:ASN:O	2:E:363:LEU:HA	2.14	0.47
4:I:341:LEU:HG	4:I:343:ILE:CD1	2.45	0.47
1:A:144:VAL:HG21	1:A:148:ILE:HD11	1.96	0.47
2:B:255:THR:HG22	2:B:256:CYS:O	2.14	0.47
1:A:374:VAL:HG11	1:A:383:MET:HG3	1.96	0.47
2:K:245:VAL:HG22	2:K:301:ARG:HG2	1.96	0.47
2:G:154:ILE:HB	2:G:155:PRO:CD	2.42	0.47
2:G:176:PRO:C	2:G:178:ALA:N	2.67	0.47
2:K:124:SER:HB3	2:K:127:ASP:OD2	2.14	0.47
2:E:341:LEU:HD12	2:E:342:LEU:H	1.79	0.47
2:G:269:ARG:C	2:G:271:ASP:N	2.68	0.47
2:G:301:ARG:HH12	2:G:304:LEU:HD11	1.80	0.47
2:B:135:ARG:HD2	2:B:138:GLN:HG3	1.96	0.47
2:B:180:PHE:CE2	3:D:2:BTK:HAF	2.50	0.47
2:G:263:PHE:HB3	2:G:264:PRO:HD2	1.96	0.47
2:K:235:ARG:HG2	2:K:244:LEU:HD23	1.97	0.47
1:A:318:LEU:HD22	1:A:343:ILE:HB	1.96	0.47
2:E:131:LEU:HA	2:E:131:LEU:HD23	1.69	0.47
2:E:305:HIS:ND1	2:E:306:VAL:N	2.63	0.47
4:I:341:LEU:HD12	4:I:342:LEU:H	1.81	0.47
2:K:154:ILE:HG23	2:K:155:PRO:HD2	1.95	0.47
2:K:210:HIS:ND1	2:K:233:LEU:HB3	2.30	0.47
1:A:321:SER:HA	1:A:348:VAL:HG21	1.97	0.46
4:I:309:PHE:CE2	4:I:330:LEU:HB3	2.49	0.46
2:B:190:LYS:N	2:B:191:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:304:LEU:HD21	2:B:303:LEU:CD1	2.44	0.46
4:I:150:THR:N	4:I:151:PRO:HD2	2.30	0.46
2:K:231:ASP:O	2:K:233:LEU:N	2.47	0.46
2:G:175:TYR:N	2:G:175:TYR:CD1	2.78	0.46
2:G:241:ALA:HA	2:G:244:LEU:HD13	1.98	0.46
4:I:188:ASN:OD1	4:I:190:LYS:HB2	2.15	0.46
2:K:248:HIS:HD2	3:L:2:BTK:HAFA	1.79	0.46
2:B:200:TYR:CE2	2:B:272:VAL:HG11	2.50	0.46
2:E:268:ILE:O	2:E:272:VAL:HG23	2.16	0.46
1:A:174:PRO:HG2	1:A:175:TYR:CD1	2.51	0.46
2:B:325:GLU:O	3:D:2:BTK:HA	2.15	0.46
4:I:132:ILE:O	4:I:135:ARG:N	2.45	0.46
1:A:261:ARG:NH1	1:A:261:ARG:HG2	2.30	0.46
2:G:279:ARG:HA	2:G:285:GLY:O	2.16	0.46
2:G:292:VAL:HG12	3:H:2:BTK:CD	2.44	0.46
2:G:347:LEU:O	2:G:348:VAL:CG1	2.64	0.46
2:K:225:LEU:HD21	2:K:234:GLU:HG2	1.97	0.46
2:G:178:ALA:O	2:G:181:GLU:HB2	2.16	0.46
2:G:286:VAL:HG23	2:G:287:VAL:N	2.31	0.46
4:I:228:GLN:HB2	4:I:327:PHE:CD2	2.51	0.46
1:A:347:LEU:HD12	1:A:352:ALA:CB	2.41	0.46
2:G:280:CYS:SG	2:G:283:CYS:SG	3.12	0.46
2:G:309:PHE:N	2:G:310:PRO:CD	2.79	0.46
2:G:342:LEU:HD22	2:G:344:ASN:HB2	1.95	0.46
2:K:141:VAL:CG2	2:K:223:LEU:HD23	2.46	0.46
2:G:264:PRO:HD2	2:G:267:ASP:OD2	2.16	0.45
4:I:147:GLY:O	4:I:151:PRO:HD3	2.16	0.45
4:I:364:GLY:O	4:I:365:ASP:C	2.54	0.45
2:K:143:MET:CE	2:K:331:THR:HG22	2.46	0.45
2:B:367:VAL:O	2:B:371:GLU:HG3	2.16	0.45
2:B:228:GLN:NE2	6:B:1396:GOL:H31	2.31	0.45
3:J:0:ARG:CG	3:J:0:ARG:NH1	2.63	0.45
2:G:141:VAL:HG22	2:G:223:LEU:HD23	1.97	0.45
2:G:282:VAL:N	2:G:283:CYS:C	2.70	0.45
2:G:286:VAL:CG2	2:G:287:VAL:N	2.77	0.45
1:A:135:ARG:C	1:A:137:CYS:N	2.69	0.45
1:A:154:ILE:HG23	1:A:155:PRO:HD2	1.97	0.45
2:B:214:ARG:NE	2:B:218:ASP:OD2	2.49	0.45
2:E:125:LEU:HG	2:E:376:LEU:CD1	2.47	0.45
4:I:127:ASP:O	4:I:130:GLU:HB3	2.17	0.45
4:I:188:ASN:OD1	4:I:191:PRO:HD3	2.17	0.45
4:I:386:LEU:CD1	4:I:390:GLU:HG2	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:I:1394:GOL:H12	3:J:2:BTK:HAA	1.99	0.45
1:A:128:VAL:O	1:A:131:LEU:HB2	2.16	0.45
1:A:168:LEU:O	1:A:171:TYR:O	2.35	0.45
2:G:241:ALA:HA	2:G:244:LEU:CD1	2.47	0.45
4:I:195:LEU:O	4:I:199:LEU:CD1	2.64	0.45
2:K:349:GLY:O	2:K:353:TRP:N	2.46	0.45
1:A:168:LEU:HD21	1:A:176:PRO:HA	1.98	0.45
2:E:124:SER:O	2:E:125:LEU:C	2.51	0.45
2:E:173:LEU:HA	2:E:174:PRO:HD2	1.75	0.45
2:G:268:ILE:HD11	2:G:289:PRO:HG3	1.99	0.45
4:I:314:LEU:CD1	4:I:339:PRO:HB2	2.47	0.45
2:K:351:LEU:CD2	2:K:351:LEU:N	2.77	0.45
1:A:321:SER:O	1:A:348:VAL:HG21	2.17	0.45
2:B:268:ILE:HD12	2:B:289:PRO:HG3	2.00	0.45
1:A:175:TYR:HB2	1:A:176:PRO:HD2	1.99	0.44
1:A:320:THR:HG21	1:A:322:LEU:HD23	1.99	0.44
2:E:349:GLY:HA2	2:E:353:TRP:CH2	2.52	0.44
2:G:201:PRO:C	2:G:203:ASN:H	2.20	0.44
2:G:268:ILE:HB	2:G:278:PRO:HG2	1.99	0.44
4:I:148:ILE:CG2	4:I:318:LEU:O	2.65	0.44
4:I:147:GLY:HA3	4:I:319:GLY:O	2.17	0.44
4:I:141:VAL:HG21	4:I:312:ALA:HB2	1.98	0.44
4:I:342:LEU:HD11	4:I:344:ASN:HB2	2.00	0.44
2:B:264:PRO:HG2	2:B:267:ASP:HB2	1.99	0.44
2:B:269:ARG:O	2:B:273:MET:HG2	2.17	0.44
2:E:365:ASP:OD1	2:E:367:VAL:N	2.48	0.44
3:J:0:ARG:HB3	3:J:1:THR:H	1.71	0.44
2:K:288:LYS:HD3	2:K:288:LYS:O	2.17	0.44
1:A:259:CYS:O	1:A:260:GLN:HB2	2.17	0.44
2:E:317:ILE:O	2:E:342:LEU:HD12	2.18	0.44
2:G:189:PRO:C	2:G:191:PRO:CD	2.86	0.44
2:K:242:SER:HA	2:K:301:ARG:NH2	2.32	0.44
1:A:124:SER:O	1:A:127:ASP:HB2	2.17	0.44
2:B:190:LYS:N	2:B:191:PRO:CD	2.81	0.44
1:A:292:VAL:HG11	1:A:298:LEU:CD2	2.48	0.44
1:A:353:TRP:O	1:A:355:PRO:HD3	2.17	0.44
2:B:277:VAL:HA	2:B:278:PRO:HD3	1.78	0.44
4:I:211:TYR:HA	4:I:214:ARG:HB3	1.99	0.44
2:E:182:LEU:HB3	2:K:303:LEU:HD13	2.00	0.44
2:K:142:VAL:HA	2:K:316:LEU:O	2.18	0.44
1:A:170:GLN:HB3	1:A:171:TYR:HD1	1.83	0.44
4:I:127:ASP:O	4:I:131:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:123:LEU:HD12	2:K:123:LEU:HA	1.84	0.44
2:G:216:LEU:HD23	2:G:216:LEU:HA	1.76	0.44
2:K:366:VAL:HG23	2:K:367:VAL:N	2.31	0.44
2:E:135:ARG:NH2	2:E:219:LYS:O	2.51	0.43
3:F:5:ALA:O	3:F:6:ARG:C	2.56	0.43
2:G:309:PHE:CZ	2:G:330:LEU:HB3	2.53	0.43
1:A:124:SER:H	1:A:127:ASP:HB2	1.83	0.43
1:A:264:PRO:O	1:A:267:ASP:HB2	2.18	0.43
2:E:216:LEU:HD22	2:E:221:LEU:HB2	2.00	0.43
4:I:233:LEU:HA	4:I:236:VAL:CG2	2.48	0.43
4:I:363:LEU:HD12	4:I:363:LEU:N	2.33	0.43
4:I:126:GLN:HA	4:I:376:LEU:HD23	1.99	0.43
2:B:381:GLU:HG3	2:B:384:ARG:NH1	2.33	0.43
2:E:133:ARG:HD2	2:E:377:LEU:O	2.18	0.43
3:F:1:THR:O	3:F:3:GLN:HG2	2.18	0.43
2:G:121:GLY:HA2	2:G:122:LYS:HA	1.55	0.43
4:I:222:LEU:HD12	4:I:223:LEU:N	2.33	0.43
4:I:200:TYR:HE2	4:I:269:ARG:HG3	1.82	0.43
4:I:288:LYS:HA	4:I:289:PRO:HD2	1.84	0.43
4:I:144:VAL:HG12	4:I:318:LEU:HG	2.01	0.43
2:K:213:LEU:HD13	2:K:225:LEU:CD1	2.48	0.43
2:K:293:PHE:O	2:K:296:GLU:HB2	2.19	0.43
1:A:228:GLN:OE1	1:A:327:PHE:CE2	2.71	0.43
2:K:298:LEU:HD11	2:K:326:PRO:HD2	1.99	0.43
4:I:280:CYS:HA	4:I:281:PRO:HD2	1.80	0.43
2:B:239:ILE:HA	2:B:240:PRO:HD2	1.91	0.43
2:G:175:TYR:CB	2:G:176:PRO:CD	2.88	0.43
1:A:235:ARG:HD2	1:A:239:ILE:O	2.19	0.43
1:A:321:SER:O	1:A:348:VAL:HG22	2.18	0.43
2:G:236:VAL:HG12	2:G:236:VAL:O	2.18	0.43
1:A:280:CYS:HB3	1:A:283:CYS:HB2	2.00	0.43
2:G:317:ILE:C	2:G:317:ILE:HD13	2.39	0.43
3:H:5:ALA:O	3:H:6:ARG:C	2.57	0.43
4:I:349:GLY:O	4:I:352:ALA:N	2.52	0.43
2:K:228:GLN:HE22	2:K:324:VAL:CG1	2.32	0.43
1:A:188:ASN:OD1	1:A:191:PRO:HD3	2.18	0.42
2:B:325:GLU:HB3	2:B:326:PRO:HA	2.01	0.42
2:E:259:CYS:SG	2:E:261:ARG:CG	2.99	0.42
2:G:207:ASN:OD1	2:G:209:THR:HB	2.19	0.42
2:G:338:VAL:HA	2:G:339:PRO:HD2	1.94	0.42
1:A:226:TYR:OH	1:A:305:HIS:HA	2.19	0.42
2:B:392:GLY:C	2:B:394:LEU:N	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:142:VAL:HG12	2:E:143:MET:N	2.34	0.42
2:E:243:LYS:HZ2	2:E:243:LYS:HG3	1.72	0.42
2:E:317:ILE:C	2:E:318:LEU:HD23	2.39	0.42
2:G:393:LYS:O	2:G:394:LEU:HD12	2.18	0.42
4:I:347:LEU:HD12	4:I:348:VAL:N	2.28	0.42
2:B:177:GLU:O	2:B:178:ALA:C	2.57	0.42
2:E:362:GLN:HA	2:E:362:GLN:NE2	2.33	0.42
4:I:219:LYS:HD2	4:I:379:TRP:CZ2	2.53	0.42
1:A:283:CYS:HB3	1:A:285:GLY:H	1.83	0.42
2:G:317:ILE:HD13	2:G:342:LEU:HD23	2.00	0.42
2:K:143:MET:HB3	2:K:327:PHE:CZ	2.55	0.42
2:E:180:PHE:CD2	3:F:2:BTK:HAF	2.53	0.42
2:G:269:ARG:C	2:G:271:ASP:H	2.22	0.42
2:K:228:GLN:HB2	2:K:248:HIS:CD2	2.54	0.42
1:A:128:VAL:O	1:A:129:ALA:C	2.57	0.42
2:G:294:PHE:HA	3:H:2:BTK:O	2.19	0.42
4:I:147:GLY:O	4:I:151:PRO:HD2	2.19	0.42
2:B:214:ARG:HE	2:B:218:ASP:CG	2.23	0.42
2:B:235:ARG:HD2	2:B:239:ILE:O	2.19	0.42
4:I:283:CYS:C	4:I:284:THR:HG22	2.38	0.42
2:K:142:VAL:HB	2:K:225:LEU:HD12	2.02	0.42
1:A:298:LEU:HB3	1:A:299:PRO:CD	2.50	0.42
4:I:340:ARG:NH1	4:I:356:ARG:NH1	2.67	0.42
2:G:190:LYS:N	2:G:191:PRO:CD	2.83	0.42
4:I:128:VAL:HA	4:I:131:LEU:HD12	2.02	0.42
2:B:233:LEU:HD23	2:B:233:LEU:HA	1.86	0.42
2:E:289:PRO:O	2:E:291:ILE:N	2.48	0.42
2:G:150:THR:N	2:G:151:PRO:CD	2.83	0.42
2:K:228:GLN:CD	6:K:1395:GOL:H2	2.40	0.42
2:B:318:LEU:CD2	2:B:343:ILE:HB	2.50	0.41
2:G:141:VAL:CG2	2:G:223:LEU:HD23	2.50	0.41
2:K:349:GLY:O	2:K:352:ALA:HB3	2.20	0.41
1:A:121:GLY:HA2	1:A:122:LYS:HA	1.56	0.41
2:K:233:LEU:HD23	2:K:233:LEU:HA	1.61	0.41
1:A:309:PHE:N	1:A:310:PRO:CD	2.84	0.41
2:B:320:THR:HG23	6:B:1396:GOL:C3	2.51	0.41
2:G:123:LEU:O	2:G:360:VAL:HG22	2.20	0.41
2:G:374:VAL:HG11	2:G:383:MET:HG3	2.03	0.41
2:K:291:ILE:HG22	2:K:292:VAL:H	1.83	0.41
1:A:180:PHE:CE2	3:C:2:BTK:CAA	3.03	0.41
2:G:182:LEU:N	2:G:183:PRO:CD	2.83	0.41
2:E:124:SER:H	2:E:127:ASP:HB2	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:225:LEU:HD12	4:I:226:TYR:N	2.36	0.41
1:A:325:GLU:OE1	1:A:325:GLU:HA	2.21	0.41
2:B:154:ILE:HA	2:B:155:PRO:HD3	1.91	0.41
2:B:320:THR:HG22	2:B:322:LEU:N	2.18	0.41
2:E:340:ARG:CZ	2:E:356:ARG:HD2	2.50	0.41
2:K:309:PHE:HB3	2:K:333:ALA:O	2.20	0.41
2:B:177:GLU:O	2:B:179:ILE:N	2.53	0.41
2:E:171:TYR:HB3	2:E:173:LEU:CD2	2.51	0.41
2:E:217:HIS:CE1	2:E:243:LYS:HZ2	2.39	0.41
2:G:215:LEU:HD23	2:G:379:TRP:CE3	2.55	0.41
4:I:235:ARG:HD2	4:I:241:ALA:HB2	2.02	0.41
1:A:180:PHE:CZ	3:C:2:BTK:HAAB	2.56	0.41
2:E:151:PRO:HG2	2:E:207:ASN:HD21	1.82	0.41
4:I:192:PHE:CD1	4:I:192:PHE:C	2.94	0.41
2:B:347:LEU:HD12	2:B:347:LEU:HA	1.88	0.41
2:E:335:ARG:HB2	2:E:335:ARG:HE	1.72	0.41
2:G:215:LEU:HD13	2:G:386:LEU:HD22	2.02	0.41
4:I:214:ARG:HD3	4:I:237:SER:O	2.20	0.41
4:I:302:PHE:C	4:I:304:LEU:N	2.74	0.41
1:A:154:ILE:CG2	1:A:155:PRO:HD2	2.50	0.40
2:G:274:ALA:O	2:G:276:ARG:HG3	2.20	0.40
2:K:294:PHE:HA	3:L:2:BTK:HB2	2.03	0.40
1:A:168:LEU:CD2	1:A:176:PRO:HA	2.52	0.40
1:A:349:GLY:HA3	1:A:350:PRO:HD2	1.93	0.40
1:A:219:LYS:HE3	1:A:379:TRP:CD2	2.56	0.40
2:B:137:CYS:SG	2:B:314:LEU:HB2	2.60	0.40
2:E:208:VAL:HG23	2:E:383:MET:HE2	2.02	0.40
2:E:248:HIS:ND1	3:F:2:BTK:CAN	2.84	0.40
2:G:263:PHE:CB	2:G:264:PRO:CD	2.98	0.40
4:I:284:THR:OG1	4:I:284:THR:O	2.33	0.40
4:I:304:LEU:HA	4:I:304:LEU:HD23	1.68	0.40
4:I:348:VAL:C	4:I:352:ALA:HB2	2.42	0.40
2:K:325:GLU:OE1	2:K:326:PRO:HA	2.21	0.40
2:K:375:GLU:HG2	2:K:380:THR:OG1	2.21	0.40
4:I:240:PRO:HG2	4:I:243:LYS:HB2	2.03	0.40
1:A:186:PHE:CE2	2:E:300:GLN:HG3	2.57	0.40
2:B:374:VAL:HG13	2:B:379:TRP:HB2	2.03	0.40
2:E:225:LEU:HD12	2:E:226:TYR:N	2.36	0.40
2:K:349:GLY:HA3	2:K:350:PRO:HD3	1.75	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	267/275 (97%)	250 (94%)	14 (5%)	3 (1%)	21	66
2	B	261/275 (95%)	237 (91%)	20 (8%)	4 (2%)	15	56
2	E	258/275 (94%)	234 (91%)	24 (9%)	0	100	100
2	G	247/275 (90%)	218 (88%)	28 (11%)	1 (0%)	43	85
2	K	186/275 (68%)	174 (94%)	12 (6%)	0	100	100
3	C	4/7 (57%)	4 (100%)	0	0	100	100
3	D	4/7 (57%)	4 (100%)	0	0	100	100
3	F	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
3	H	4/7 (57%)	4 (100%)	0	0	100	100
3	J	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
3	L	4/7 (57%)	4 (100%)	0	0	100	100
4	I	247/275 (90%)	221 (90%)	23 (9%)	3 (1%)	19	63
All	All	1490/1692 (88%)	1356 (91%)	123 (8%)	11 (1%)	30	76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	159	SER
2	G	154	ILE
4	I	201	PRO
1	A	136	ALA
2	B	393	LYS
2	B	178	ALA
1	A	172	ASP
1	A	201	PRO
2	B	147	GLY
4	I	191	PRO
4	I	200	TYR

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	234/238 (98%)	228 (97%)	6 (3%)	59	91
2	B	227/238 (95%)	213 (94%)	14 (6%)	26	66
2	E	227/238 (95%)	213 (94%)	14 (6%)	26	66
2	G	212/238 (89%)	200 (94%)	12 (6%)	29	70
2	K	160/238 (67%)	149 (93%)	11 (7%)	22	61
3	C	5/5 (100%)	5 (100%)	0	100	100
3	D	5/5 (100%)	4 (80%)	1 (20%)	2	9
3	F	5/5 (100%)	4 (80%)	1 (20%)	2	9
3	H	5/5 (100%)	4 (80%)	1 (20%)	2	9
3	J	5/5 (100%)	3 (60%)	2 (40%)	0	0
3	L	5/5 (100%)	3 (60%)	2 (40%)	0	0
4	I	210/238 (88%)	190 (90%)	20 (10%)	12	41
All	All	1300/1458 (89%)	1216 (94%)	84 (6%)	24	63

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	170	GLN
1	A	208	VAL
1	A	237	SER
1	A	347	LEU
1	A	365	ASP
2	B	138	GLN
2	B	156	ASP
2	B	194	THR
2	B	224	ARG
2	B	248	HIS
2	B	253	SER
2	B	258	VAL
2	B	288	LYS
2	B	298	LEU

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Mol	Chain	Res	Type
2	B	316	LEU
2	B	346	ASP
2	B	351	LEU
2	B	365	ASP
2	B	391	THR
3	D	1	THR
2	E	156	ASP
2	E	168	LEU
2	E	188	ASN
2	E	203	ASN
2	E	215	LEU
2	E	225	LEU
2	E	227	THR
2	E	235	ARG
2	E	283	CYS
2	E	291	ILE
2	E	320	THR
2	E	357	SER
2	E	380	THR
2	E	391	THR
3	F	0	ARG
2	G	124	SER
2	G	148	ILE
2	G	177	GLU
2	G	184	PHE
2	G	225	LEU
2	G	244	LEU
2	G	256	CYS
2	G	263	PHE
2	G	286	VAL
2	G	317	ILE
2	G	320	THR
2	G	342	LEU
3	H	6	ARG
4	I	126	GLN
4	I	148	ILE
4	I	154	ILE
4	I	199	LEU
4	I	227	THR
4	I	231	ASP
4	I	237	SER
4	I	246	GLU

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Mol	Chain	Res	Type
4	I	266	GLU
4	I	275	ASP
4	I	284	THR
4	I	318	LEU
4	I	321	SER
4	I	329	SER
4	I	354	HIS
4	I	358	ARG
4	I	365	ASP
4	I	371	GLU
4	I	376	LEU
4	I	389	ARG
3	J	0	ARG
3	J	4	THR
2	K	235	ARG
2	K	288	LYS
2	K	290	ASP
2	K	292	VAL
2	K	293	PHE
2	K	346	ASP
2	K	347	LEU
2	K	354	HIS
2	K	363	LEU
2	K	367	VAL
2	K	380	THR
3	L	3	GLN
3	L	4	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	188	ASN
2	E	203	ASN
2	G	354	HIS
2	K	228	GLN
2	K	248	HIS
2	K	344	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	BTK	C	2	3	13,13,14	4.41	2 (15%)	12,14,16	1.16	2 (16%)
3	BTK	D	2	3	13,13,14	4.29	2 (15%)	12,14,16	1.22	2 (16%)
3	BTK	F	2	3	13,13,14	4.72	2 (15%)	12,14,16	2.10	4 (33%)
3	BTK	H	2	3	13,13,14	3.57	3 (23%)	12,14,16	1.63	4 (33%)
3	BTK	J	2	3	13,13,14	4.47	2 (15%)	12,14,16	1.31	2 (16%)
3	BTK	L	2	3	13,13,14	4.42	2 (15%)	12,14,16	1.71	2 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BTK	C	2	3	-	0/11/13/15	0/0/0/0
3	BTK	D	2	3	-	0/11/13/15	0/0/0/0
3	BTK	F	2	3	-	0/11/13/15	0/0/0/0
3	BTK	H	2	3	-	0/11/13/15	0/0/0/0
3	BTK	J	2	3	-	0/11/13/15	0/0/0/0
3	BTK	L	2	3	-	0/11/13/15	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	BTK	O-C	16.69	1.22	1.11
3	J	2	BTK	O-C	15.78	1.22	1.11
3	L	2	BTK	O-C	15.62	1.22	1.11
3	C	2	BTK	O-C	15.54	1.22	1.11
3	D	2	BTK	O-C	15.00	1.21	1.11
3	H	2	BTK	O-C	11.70	1.19	1.11
3	H	2	BTK	OAD-CAN	-4.00	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	BTK	CAN-NZ	-3.35	1.25	1.33
3	H	2	BTK	CAN-NZ	-3.07	1.26	1.33
3	J	2	BTK	CAN-NZ	-3.01	1.26	1.33
3	C	2	BTK	CAN-NZ	-2.82	1.26	1.33
3	F	2	BTK	CAN-NZ	-2.65	1.27	1.33
3	L	2	BTK	CAN-NZ	-2.59	1.27	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2	BTK	C-CA-N	-4.42	109.41	113.83
3	F	2	BTK	CE-NZ-CAN	4.09	131.15	122.81
3	F	2	BTK	CD-CE-NZ	-3.44	101.95	112.20
3	F	2	BTK	C-CA-N	-3.40	110.43	113.83
3	J	2	BTK	C-CA-N	-2.98	110.85	113.83
3	H	2	BTK	OAD-CAN-NZ	-2.70	117.62	122.94
3	L	2	BTK	CAF-CAJ-CAN	-2.67	107.63	113.38
3	C	2	BTK	CE-NZ-CAN	2.54	127.98	122.81
3	D	2	BTK	C-CA-N	-2.46	111.37	113.83
3	H	2	BTK	OAD-CAN-CAJ	2.44	126.61	121.92
3	J	2	BTK	CD-CE-NZ	-2.20	105.66	112.20
3	H	2	BTK	CD-CE-NZ	-2.19	105.67	112.20
3	F	2	BTK	CAJ-CAN-NZ	-2.11	112.66	116.48
3	C	2	BTK	C-CA-N	-2.06	111.78	113.83
3	D	2	BTK	CAF-CAJ-CAN	-2.04	108.98	113.38
3	H	2	BTK	CE-NZ-CAN	2.04	126.96	122.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	1396	-	5,5,5	0.28	0	5,5,5	0.56	0
6	GOL	E	1395	-	5,5,5	0.27	0	5,5,5	0.22	0
6	GOL	E	1396	-	5,5,5	0.32	0	5,5,5	0.30	0
6	GOL	G	1396	-	5,5,5	0.34	0	5,5,5	0.27	0
6	GOL	I	1394	-	5,5,5	0.35	0	5,5,5	0.37	0
6	GOL	K	1395	-	5,5,5	0.29	0	5,5,5	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	1396	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1395	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1396	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1396	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1394	-	-	0/4/4/4	0/0/0/0
6	GOL	K	1395	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9
1	A	270/275 (98%)	-0.29	1 (0%) 90 54	17, 30, 61, 85	1 (0%)
2	B	264/275 (96%)	-0.23	3 (1%) 77 36	17, 31, 64, 105	0
2	E	263/275 (95%)	-0.24	2 (0%) 83 42	21, 36, 64, 97	1 (0%)
2	G	252/275 (91%)	0.00	5 (1%) 62 27	19, 42, 76, 87	0
2	K	191/275 (69%)	0.18	10 (5%) 26 13	29, 55, 90, 116	1 (0%)
3	C	6/7 (85%)	-0.22	0 100 100	28, 32, 44, 68	0
3	D	6/7 (85%)	0.62	1 (16%) 2 2	35, 39, 52, 88	0
3	F	6/7 (85%)	0.50	1 (16%) 2 2	45, 47, 79, 79	0
3	H	6/7 (85%)	0.40	0 100 100	56, 63, 81, 97	0
3	J	6/7 (85%)	0.74	1 (16%) 2 2	61, 74, 103, 139	0
3	L	6/7 (85%)	2.46	3 (50%) 0 0	86, 90, 97, 111	0
4	I	251/275 (91%)	0.22	11 (4%) 33 16	29, 55, 95, 130	0
All	All	1527/1692 (90%)	-0.05	38 (2%) 54 24	17, 40, 80, 139	3 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	6	ARG	6.0
2	G	282	VAL	5.1
2	K	294	PHE	4.5
2	K	287	VAL	4.4
2	G	281	PRO	4.2
4	I	368	HIS	4.1
2	K	323	GLU	4.0
2	K	394	LEU	3.9
2	K	353	TRP	3.8
4	I	153	GLY	3.6
4	I	125	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	K	123	LEU	3.3
4	I	392	GLY	3.2
3	L	5	ALA	3.2
3	J	6	ARG	3.2
2	G	121	GLY	3.1
2	K	292	VAL	3.0
2	E	168	LEU	3.0
4	I	137	CYS	2.8
1	A	165	TYR	2.7
2	G	200	TYR	2.7
2	B	395	ASP	2.6
2	K	295	GLY	2.4
2	B	160	PRO	2.4
2	K	351	LEU	2.3
3	L	0	ARG	2.3
3	F	6	ARG	2.3
4	I	198	GLU	2.3
2	B	277	VAL	2.2
2	K	289	PRO	2.2
2	E	388	GLN	2.2
4	I	134	ALA	2.1
3	D	6	ARG	2.1
4	I	136	ALA	2.1
4	I	202	ALA	2.1
4	I	336	SER	2.1
2	G	193	PHE	2.1
4	I	347	LEU	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	BTK	L	2	14/15	0.39	1.03	70,82,88,94	0
3	BTK	J	2	14/15	0.22	0.45	44,52,61,64	0
3	BTK	D	2	14/15	0.20	0.38	24,27,32,33	0
3	BTK	C	2	14/15	0.17	0.35	16,23,25,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BTK	H	2	14/15	0.18	0.03	38,43,52,53	0
3	BTK	F	2	14/15	0.15	-0.24	27,32,37,40	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	K	1395	6/6	0.52	7.54	64,66,68,69	0
6	GOL	E	1395	6/6	0.26	4.12	42,46,50,53	0
6	GOL	E	1396	6/6	0.47	3.31	72,74,79,87	0
6	GOL	G	1396	6/6	0.22	1.83	43,46,49,51	0
6	GOL	I	1394	6/6	0.26	0.78	38,51,52,59	0
5	ZN	E	1397	1/1	0.17	0.63	37,37,37,37	0
6	GOL	B	1396	6/6	0.19	0.61	26,29,33,34	0
5	ZN	I	1395	1/1	0.14	-0.07	36,36,36,36	0
5	ZN	G	1395	1/1	0.20	-0.52	104,104,104,104	0
5	ZN	B	1397	1/1	0.09	-1.06	47,47,47,47	0
5	ZN	A	1395	1/1	0.11	-1.28	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.