



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 3AQM / pdb_00003aqm
Title : Structure of bacterial protein (form II)
Authors : Toh, Y.; Takeshita, D.; Tomita , K.
Deposited on : 2010-11-09
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

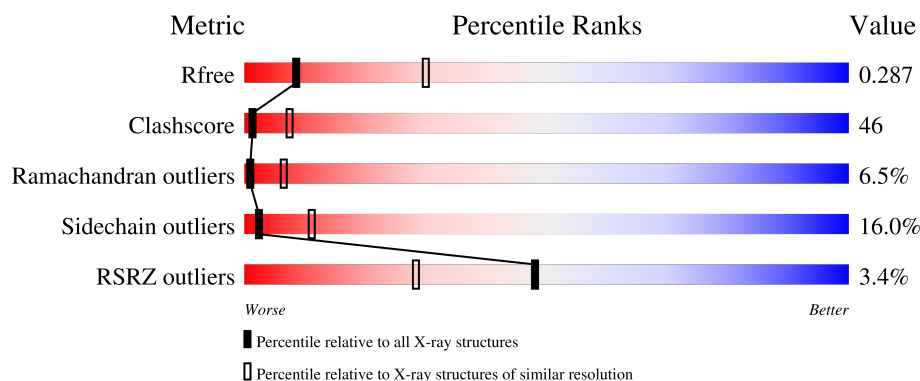
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	415	4% 31% 48% 13% 7%
1	B	415	3% 31% 46% 15% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6332 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 Poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3165	2022	569	560	14			
1	B	388	Total	C	N	O	S	0	0	0
			3165	2022	569	560	14			

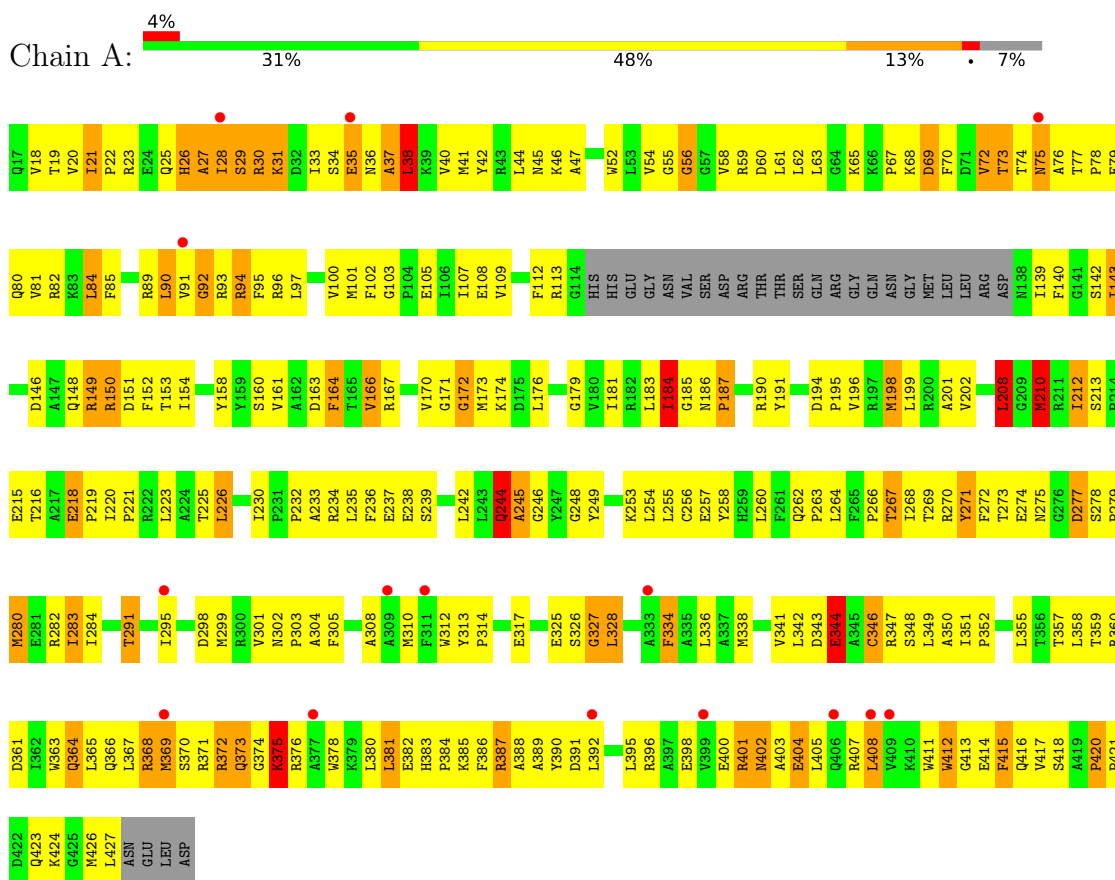
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

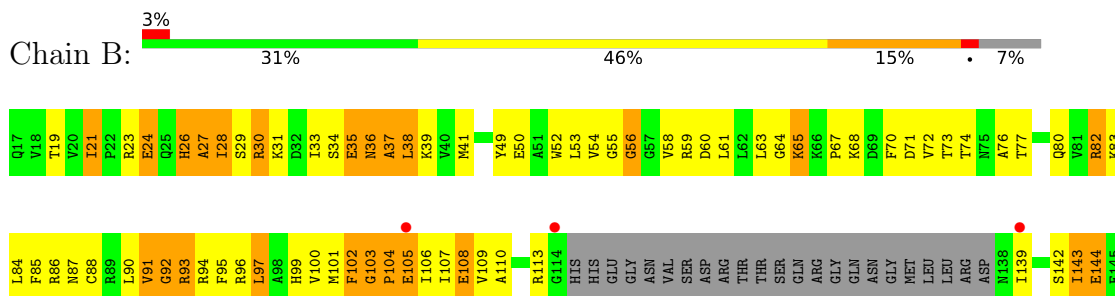
3 Residue-property plots

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: Poly(A) polymerase



• Molecule 1: Poly(A) polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	133.25Å 133.25Å 176.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 3.15 29.80 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.80-3.15) 97.7 (29.80-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.270 , 0.287 0.290 , 0.287	Depositor DCC
R_{free} test set	1364 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	91.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6332	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.51	0/3234	1.10	23/4370 (0.5%)
1	B	0.51	0/3234	1.13	32/4370 (0.7%)
All	All	0.51	0/6468	1.11	55/8740 (0.6%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ALA	N-CA-C	-13.61	96.67	113.28
1	A	37	ALA	N-CA-C	-12.47	96.79	112.88
1	A	29	SER	N-CA-C	-10.27	90.69	108.56
1	B	420	PRO	N-CA-C	9.54	122.34	110.70
1	B	376	ARG	N-CA-C	-9.51	101.44	113.23
1	A	208	LEU	N-CA-C	-8.79	99.19	110.53
1	B	326	SER	N-CA-C	-8.74	102.19	112.86
1	A	38	LEU	N-CA-C	-8.33	101.73	112.23
1	A	21	ILE	CA-C-N	7.53	128.12	120.14
1	A	21	ILE	C-N-CA	7.53	128.12	120.14
1	B	102	PHE	N-CA-C	-7.23	102.39	112.45
1	B	419	ALA	CA-C-N	7.20	127.79	120.38
1	B	419	ALA	C-N-CA	7.20	127.79	120.38
1	B	393	LEU	N-CA-C	-7.06	103.63	111.82
1	A	19	THR	N-CA-C	7.02	118.72	111.14
1	A	344	GLU	N-CA-C	-6.90	102.34	111.24
1	B	301	VAL	N-CA-C	6.66	118.30	108.45
1	B	54	VAL	N-CA-C	6.58	118.98	108.85
1	B	36	ASN	N-CA-C	6.50	119.36	110.06
1	B	405	LEU	N-CA-C	-6.45	104.46	112.72
1	B	103	GLY	N-CA-C	-6.45	99.19	112.34
1	B	406	GLN	N-CA-C	-6.41	105.18	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	GLY	N-CA-C	6.23	121.56	113.27
1	A	245	ALA	N-CA-C	6.17	123.94	110.80
1	A	373	GLN	N-CA-C	6.15	117.98	110.41
1	A	184	ILE	N-CA-C	5.97	121.76	109.34
1	B	392	LEU	N-CA-C	-5.90	105.17	112.90
1	B	282	ARG	N-CA-C	-5.88	105.77	113.12
1	B	367	LEU	N-CA-C	-5.86	104.89	112.68
1	B	19	THR	N-CA-C	5.80	117.27	111.07
1	A	54	VAL	N-CA-C	5.68	118.32	108.95
1	A	420	PRO	N-CA-C	5.65	117.60	110.70
1	A	210	MET	N-CA-C	5.64	118.43	110.14
1	B	143	ILE	N-CA-C	5.64	116.42	110.72
1	B	347	ARG	N-CA-C	-5.60	105.18	112.23
1	A	271	TYR	N-CA-C	5.55	120.16	113.17
1	B	404	GLU	N-CA-C	-5.54	105.87	113.30
1	B	297	ASN	N-CA-C	-5.45	104.84	112.25
1	A	412	TRP	N-CA-C	-5.41	106.38	112.87
1	A	35	GLU	N-CA-C	-5.34	102.88	110.35
1	B	247	TYR	N-CA-C	-5.29	105.88	114.09
1	A	392	LEU	N-CA-C	-5.28	105.98	112.90
1	A	298	ASP	N-CA-C	5.21	121.89	110.80
1	A	142	SER	N-CA-C	5.17	116.99	110.33
1	B	315	LEU	N-CA-C	-5.15	105.56	111.07
1	B	208	LEU	N-CA-C	-5.14	103.61	110.55
1	B	194	ASP	CA-C-N	5.14	125.18	119.32
1	B	194	ASP	C-N-CA	5.14	125.18	119.32
1	B	144	GLU	N-CA-C	-5.13	105.77	111.36
1	A	218	GLU	CA-C-N	5.13	125.17	119.32
1	A	218	GLU	C-N-CA	5.13	125.17	119.32
1	B	291	THR	N-CA-C	-5.11	105.70	112.34
1	B	351	ILE	CA-C-N	5.10	125.01	119.76
1	B	351	ILE	C-N-CA	5.10	125.01	119.76
1	B	336	LEU	N-CA-C	-5.05	105.24	111.40

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	3165	0	3203	304	1
1	B	3165	0	3201	286	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	6332	0	6404	585	1

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 46.

All (585) 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:B:183:LEU:HD23	1:B:184:ILE:H	1.07	1.20
1:A:95:PHE:CD1	1:A:96:ARG:HG3	1.78	1.18
1:A:149:ARG:HH11	1:A:149:ARG:HB3	1.22	1.04
1:A:372:ARG:NH1	1:A:372:ARG:HA	1.71	1.03
1:B:233:ALA:HA	1:B:350:ALA:HB3	1.43	0.98
1:A:95:PHE:CE1	1:A:96:ARG:HG3	2.00	0.96
1:B:170:VAL:HG12	1:B:171:GLY:H	1.28	0.95
1:A:378:TRP:HB3	1:B:299:MET:SD	2.07	0.94
1:A:212:ILE:H	1:A:212:ILE:HD12	1.30	0.94
1:A:375:LYS:H	1:A:375:LYS:HD2	1.32	0.94
1:B:372:ARG:HE	1:B:407:ARG:HH21	0.98	0.94
1:A:184:ILE:HG22	1:A:190:ARG:NH1	1.84	0.92
1:A:37:ALA:O	1:A:40:VAL:HG12	1.69	0.92
1:A:77:THR:H	1:A:80:GLN:HE21	0.97	0.92
1:B:374:GLY:HA3	1:B:427:LEU:HD22	1.51	0.92
1:A:372:ARG:HA	1:A:372:ARG:HH11	1.33	0.90
1:B:372:ARG:HE	1:B:407:ARG:NH2	1.69	0.90
1:A:95:PHE:CE1	1:A:96:ARG:CG	2.55	0.89
1:A:113:ARG:HG2	1:A:146:ASP:OD1	1.73	0.88
1:B:28:ILE:HG13	1:B:29:SER:H	1.37	0.88
1:B:183:LEU:HD23	1:B:184:ILE:N	1.88	0.88
1:A:196:VAL:HG21	1:A:234:ARG:NH2	1.87	0.88
1:A:271:TYR:HE1	1:A:317:GLU:HG2	1.39	0.87
1:B:244:GLN:HE22	1:B:303:PRO:HA	1.39	0.86
1:B:280:MET:HE2	1:B:314:PRO:HG3	1.56	0.86
1:B:28:ILE:HB	1:B:30:ARG:HD2	1.57	0.85
1:A:242:LEU:HD13	1:A:255:LEU:HD11	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLY:O	1:B:58:VAL:HG12	1.76	0.84
1:B:154:ILE:HD13	1:B:210:MET:HE1	1.56	0.84
1:A:184:ILE:HG22	1:A:190:ARG:HH12	1.43	0.84
1:B:103:GLY:O	1:B:105:GLU:N	2.10	0.84
1:A:302:ASN:HD21	1:A:385:LYS:NZ	1.75	0.84
1:B:184:ILE:HG22	1:B:185:GLY:N	1.92	0.84
1:B:183:LEU:HB2	1:B:216:THR:HG23	1.59	0.84
1:A:414:GLU:HB3	1:A:426:MET:HE1	1.59	0.83
1:A:262:GLN:HB3	1:A:263:PRO:HD3	1.58	0.83
1:A:218:GLU:HB3	1:A:219:PRO:HD3	1.61	0.83
1:B:352:PRO:HG2	1:B:355:LEU:HD23	1.61	0.83
1:A:149:ARG:HB3	1:A:149:ARG:NH1	1.94	0.82
1:A:195:PRO:HB2	1:A:230:ILE:HD11	1.58	0.82
1:A:95:PHE:HE1	1:A:96:ARG:HE	1.24	0.82
1:A:196:VAL:HG21	1:A:234:ARG:HH22	1.44	0.82
1:B:30:ARG:CZ	1:B:33:ILE:HD11	2.10	0.82
1:A:184:ILE:CG2	1:A:185:GLY:N	2.44	0.81
1:A:291:THR:O	1:A:295:ILE:HG12	1.81	0.80
1:B:154:ILE:HG22	1:B:176:LEU:HB2	1.64	0.80
1:A:183:LEU:HD23	1:A:184:ILE:N	1.97	0.79
1:A:77:THR:N	1:A:80:GLN:HE21	1.79	0.79
1:A:191:TYR:CE1	1:A:198:MET:HG3	2.18	0.78
1:A:184:ILE:HG22	1:A:185:GLY:H	1.48	0.78
1:A:244:GLN:O	1:A:246:GLY:N	2.13	0.78
1:A:271:TYR:HB2	1:A:280:MET:HE3	1.66	0.78
1:A:78:PRO:O	1:A:82:ARG:HG3	1.85	0.77
1:B:34:SER:O	1:B:35:GLU:C	2.27	0.77
1:A:35:GLU:OE1	1:A:105:GLU:HG3	1.84	0.76
1:A:235:LEU:HD22	1:A:264:LEU:HD21	1.67	0.76
1:B:308:ALA:HB2	1:B:359:THR:HG23	1.67	0.76
1:B:93:ARG:O	1:B:94:ARG:HB2	1.84	0.76
1:A:77:THR:H	1:A:80:GLN:NE2	1.80	0.75
1:A:28:ILE:HG23	1:A:30:ARG:HG2	1.68	0.75
1:B:34:SER:O	1:B:35:GLU:O	2.04	0.75
1:B:372:ARG:NE	1:B:407:ARG:HH21	1.81	0.75
1:A:223:LEU:O	1:A:226:LEU:HB2	1.86	0.75
1:A:75:ASN:H	1:A:75:ASN:HD22	1.35	0.74
1:A:153:THR:HG22	1:A:170:VAL:CG1	2.18	0.74
1:B:183:LEU:CD2	1:B:184:ILE:H	1.95	0.74
1:A:232:PRO:HB2	1:A:350:ALA:HB2	1.68	0.74
1:B:170:VAL:HG12	1:B:171:GLY:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:HB3	1:B:219:PRO:HD3	1.69	0.73
1:B:324:GLN:O	1:B:324:GLN:HG2	1.89	0.73
1:A:374:GLY:HA2	1:A:427:LEU:HD22	1.71	0.73
1:B:41:MET:HE2	1:B:72:VAL:CG1	2.19	0.73
1:A:153:THR:HG22	1:A:170:VAL:HG12	1.72	0.72
1:A:21:ILE:HG23	1:A:166:VAL:HG13	1.72	0.72
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.55	0.72
1:B:248:GLY:O	1:B:288:LEU:HD13	1.90	0.72
1:A:244:GLN:HE22	1:A:303:PRO:HA	1.52	0.72
1:A:218:GLU:O	1:A:221:PRO:HD2	1.90	0.71
1:B:303:PRO:HG2	1:B:355:LEU:HD11	1.71	0.71
1:B:280:MET:HE2	1:B:314:PRO:CG	2.20	0.71
1:B:352:PRO:CG	1:B:355:LEU:HD23	2.21	0.71
1:A:101:MET:O	1:A:102:PHE:HD1	1.73	0.70
1:A:308:ALA:HB2	1:A:359:THR:HG23	1.73	0.70
1:A:170:VAL:HG12	1:A:171:GLY:N	2.05	0.70
1:B:96:ARG:O	1:B:97:LEU:O	2.08	0.70
1:B:307:PHE:CD2	1:B:351:ILE:HD11	2.27	0.70
1:B:278:SER:HB2	1:B:279:PRO:CD	2.22	0.70
1:A:238:GLU:O	1:A:242:LEU:HG	1.92	0.69
1:B:97:LEU:HD11	1:B:108:GLU:HG2	1.73	0.69
1:A:223:LEU:HD23	1:A:226:LEU:HD12	1.75	0.69
1:B:95:PHE:O	1:B:96:ARG:HB3	1.93	0.69
1:B:202:VAL:HG12	1:B:254:LEU:HB3	1.75	0.69
1:B:28:ILE:HB	1:B:30:ARG:CD	2.23	0.68
1:B:36:ASN:HD22	1:B:39:LYS:HG3	1.59	0.68
1:B:287:VAL:HG23	1:B:395:LEU:CD1	2.24	0.67
1:B:144:GLU:HA	1:B:169:TYR:CD1	2.30	0.67
1:A:299:MET:SD	1:B:378:TRP:HB3	2.34	0.67
1:A:302:ASN:ND2	1:A:385:LYS:NZ	2.42	0.67
1:A:52:TRP:CZ3	1:A:160:SER:HB2	2.29	0.67
1:A:338:MET:HE3	1:A:360:ARG:HH11	1.58	0.67
1:A:82:ARG:NH1	1:A:82:ARG:HB2	2.09	0.67
1:B:233:ALA:CA	1:B:350:ALA:HB3	2.24	0.67
1:A:150:ARG:HH21	1:A:150:ARG:HG3	1.60	0.66
1:B:60:ASP:HA	1:B:63:LEU:HD12	1.77	0.66
1:B:232:PRO:HB2	1:B:350:ALA:HB2	1.77	0.66
1:B:402:ASN:ND2	1:B:404:GLU:H	1.93	0.66
1:A:26:HIS:O	1:A:26:HIS:CD2	2.48	0.66
1:A:302:ASN:HD21	1:A:385:LYS:HZ1	1.41	0.66
1:B:244:GLN:HE21	1:B:303:PRO:HB3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ARG:O	1:A:373:GLN:N	2.29	0.66
1:A:184:ILE:HG22	1:A:185:GLY:N	2.09	0.65
1:B:150:ARG:O	1:B:184:ILE:HG13	1.96	0.65
1:A:183:LEU:HD23	1:A:184:ILE:H	1.59	0.65
1:B:244:GLN:NE2	1:B:303:PRO:HA	2.10	0.65
1:A:402:ASN:C	1:A:402:ASN:HD22	2.04	0.65
1:B:278:SER:HB2	1:B:279:PRO:HD2	1.77	0.65
1:A:269:THR:HA	1:A:272:PHE:CE2	2.32	0.65
1:A:220:ILE:HB	1:A:221:PRO:HD3	1.79	0.65
1:B:280:MET:CE	1:B:314:PRO:HG3	2.27	0.64
1:A:22:PRO:HG2	1:A:25:GLN:HE21	1.61	0.64
1:A:34:SER:HB3	1:A:38:LEU:HD21	1.77	0.64
1:A:402:ASN:ND2	1:A:404:GLU:H	1.95	0.64
1:B:311:PHE:HE1	1:B:345:ALA:CB	2.10	0.64
1:A:198:MET:HG2	1:A:220:ILE:HG23	1.79	0.64
1:B:223:LEU:O	1:B:226:LEU:HB2	1.96	0.64
1:B:380:LEU:HD22	1:B:412:TRP:CH2	2.32	0.64
1:B:257:GLU:O	1:B:257:GLU:HG2	1.95	0.64
1:B:30:ARG:NE	1:B:33:ILE:HD11	2.12	0.64
1:A:325:GLU:O	1:A:325:GLU:HG2	1.97	0.63
1:A:402:ASN:HD22	1:A:403:ALA:N	1.96	0.63
1:B:385:LYS:HA	1:B:385:LYS:NZ	2.14	0.63
1:A:418:SER:C	1:A:423:GLN:HE21	2.06	0.63
1:A:40:VAL:HG23	1:A:85:PHE:CE2	2.33	0.63
1:A:77:THR:C	1:A:79:GLU:H	2.05	0.63
1:A:26:HIS:O	1:A:27:ALA:C	2.41	0.62
1:A:26:HIS:O	1:A:28:ILE:N	2.32	0.62
1:A:31:LYS:HE3	1:A:38:LEU:CD1	2.30	0.62
1:A:75:ASN:H	1:A:75:ASN:ND2	1.96	0.62
1:A:40:VAL:HG23	1:A:85:PHE:HE2	1.62	0.62
1:A:170:VAL:HG12	1:A:171:GLY:H	1.63	0.62
1:A:338:MET:HE3	1:A:360:ARG:NH1	2.14	0.62
1:A:79:GLU:HA	1:A:82:ARG:CZ	2.29	0.62
1:B:183:LEU:HB2	1:B:216:THR:CG2	2.29	0.62
1:B:184:ILE:CG2	1:B:185:GLY:N	2.63	0.62
1:B:278:SER:O	1:B:282:ARG:HD2	1.99	0.62
1:B:199:LEU:HD22	1:B:242:LEU:HD11	1.80	0.62
1:A:191:TYR:CD1	1:A:198:MET:HG3	2.34	0.62
1:B:27:ALA:O	1:B:28:ILE:C	2.43	0.62
1:A:196:VAL:CG2	1:A:234:ARG:HH22	2.11	0.61
1:A:77:THR:C	1:A:79:GLU:N	2.56	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:CB	1:A:82:ARG:HH11	2.12	0.61
1:B:170:VAL:HG11	1:B:184:ILE:CD1	2.30	0.61
1:B:271:TYR:HE1	1:B:317:GLU:HG2	1.66	0.61
1:A:271:TYR:CE1	1:A:317:GLU:HG2	2.30	0.61
1:B:97:LEU:CD1	1:B:108:GLU:HG2	2.29	0.61
1:B:56:GLY:HA2	1:B:59:ARG:HH12	1.65	0.61
1:B:346:CYS:HA	1:B:349:LEU:O	2.00	0.61
1:A:196:VAL:CG2	1:A:234:ARG:NH2	2.60	0.61
1:B:213:SER:HB3	1:B:216:THR:OG1	2.01	0.61
1:B:72:VAL:HG23	1:B:109:VAL:HG22	1.81	0.61
1:A:34:SER:CB	1:A:38:LEU:HD21	2.31	0.61
1:A:279:PRO:HA	1:A:282:ARG:HD3	1.82	0.61
1:A:368:ARG:NH1	1:A:380:LEU:HD11	2.15	0.61
1:B:179:GLY:CA	1:B:210:MET:HG2	2.30	0.61
1:B:37:ALA:CB	1:B:107:ILE:HG12	2.31	0.60
1:B:82:ARG:HG3	1:B:82:ARG:HH11	1.65	0.60
1:B:67:PRO:HG3	1:B:70:PHE:CZ	2.37	0.60
1:A:75:ASN:HB3	1:A:112:PHE:CE1	2.36	0.60
1:B:34:SER:HB2	1:B:38:LEU:HD21	1.83	0.60
1:B:50:GLU:HG3	1:B:52:TRP:NE1	2.15	0.60
1:B:158:TYR:O	1:B:166:VAL:HA	2.01	0.60
1:B:154:ILE:CD1	1:B:210:MET:HE1	2.27	0.60
1:B:204:PHE:O	1:B:208:LEU:HD12	2.02	0.60
1:B:262:GLN:HB3	1:B:263:PRO:HD3	1.84	0.60
1:A:223:LEU:CD2	1:A:226:LEU:HD12	2.31	0.60
1:A:271:TYR:HB2	1:A:280:MET:CE	2.30	0.60
1:A:344:GLU:O	1:A:347:ARG:HB2	2.02	0.60
1:B:268:ILE:HD11	1:B:310:MET:HB3	1.82	0.60
1:B:337:ALA:O	1:B:341:VAL:HG23	2.01	0.60
1:A:75:ASN:HB3	1:A:112:PHE:CD1	2.38	0.59
1:B:30:ARG:H	1:B:30:ARG:HD3	1.68	0.59
1:B:365:LEU:HD12	1:B:389:ALA:HB2	1.84	0.59
1:A:199:LEU:O	1:A:202:VAL:HG12	2.02	0.58
1:B:28:ILE:HG13	1:B:29:SER:N	2.15	0.58
1:B:405:LEU:C	1:B:407:ARG:H	2.09	0.58
1:A:187:PRO:O	1:A:191:TYR:HD2	1.86	0.58
1:B:184:ILE:HG22	1:B:185:GLY:H	1.68	0.58
1:B:190:ARG:HG3	1:B:190:ARG:HH11	1.67	0.58
1:B:405:LEU:C	1:B:407:ARG:N	2.59	0.58
1:A:154:ILE:HD13	1:A:210:MET:HE2	1.86	0.58
1:A:257:GLU:HG2	1:A:257:GLU:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASN:ND2	1:A:385:LYS:HZ1	2.02	0.57
1:B:41:MET:HE2	1:B:72:VAL:HG11	1.84	0.57
1:B:224:ALA:O	1:B:227:LEU:HG	2.04	0.57
1:B:407:ARG:HG2	1:B:407:ARG:HH11	1.69	0.57
1:A:35:GLU:O	1:A:37:ALA:N	2.35	0.57
1:B:143:ILE:HG23	1:B:169:TYR:HE1	1.69	0.57
1:B:202:VAL:CG1	1:B:254:LEU:HB3	2.33	0.57
1:A:184:ILE:HG23	1:A:185:GLY:N	2.18	0.57
1:A:150:ARG:HG3	1:A:150:ARG:NH2	2.17	0.57
1:B:59:ARG:NE	1:B:208:LEU:HD21	2.19	0.57
1:B:271:TYR:CE1	1:B:317:GLU:HG2	2.40	0.57
1:A:33:ILE:O	1:A:33:ILE:HG22	2.05	0.57
1:A:280:MET:HE2	1:A:314:PRO:HG3	1.86	0.57
1:A:20:VAL:HG23	1:A:167:ARG:NE	2.19	0.57
1:A:95:PHE:CE1	1:A:96:ARG:HG2	2.38	0.57
1:B:50:GLU:HG3	1:B:52:TRP:HE1	1.70	0.57
1:B:163:ASP:O	1:B:165:THR:HG23	2.05	0.57
1:B:287:VAL:HG21	1:B:309:ALA:CB	2.35	0.57
1:A:179:GLY:O	1:A:210:MET:HB2	2.05	0.56
1:A:235:LEU:HD22	1:A:264:LEU:CD2	2.36	0.56
1:A:79:GLU:HA	1:A:82:ARG:NH2	2.20	0.56
1:A:181:ILE:CD1	1:A:210:MET:HG3	2.35	0.56
1:A:190:ARG:NH1	1:A:190:ARG:HG3	2.16	0.56
1:A:220:ILE:CG2	1:A:260:LEU:HD11	2.35	0.56
1:B:101:MET:HE2	1:B:103:GLY:HA2	1.87	0.56
1:B:358:LEU:O	1:B:362:ILE:HG13	2.05	0.56
1:A:45:ASN:C	1:A:47:ALA:H	2.13	0.56
1:B:342:LEU:O	1:B:346:CYS:HB2	2.06	0.56
1:A:212:ILE:H	1:A:212:ILE:CD1	2.03	0.56
1:B:68:LYS:HE3	1:B:207:LYS:NZ	2.20	0.56
1:A:20:VAL:HG23	1:A:167:ARG:CD	2.36	0.56
1:A:368:ARG:CZ	1:A:380:LEU:HD11	2.36	0.56
1:A:299:MET:SD	1:B:378:TRP:HE3	2.28	0.56
1:A:299:MET:SD	1:B:378:TRP:CE3	2.98	0.56
1:B:179:GLY:HA2	1:B:210:MET:HG2	1.88	0.56
1:B:323:ALA:O	1:B:327:GLY:HA2	2.05	0.56
1:B:406:GLN:O	1:B:406:GLN:HG2	2.06	0.56
1:A:74:THR:HG23	1:A:76:ALA:H	1.69	0.56
1:B:26:HIS:NE2	1:B:29:SER:HB3	2.21	0.56
1:B:59:ARG:HE	1:B:208:LEU:HD21	1.71	0.56
1:B:302:ASN:OD1	1:B:385:LYS:HE3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:MET:HE2	1:A:314:PRO:CG	2.36	0.55
1:B:312:TRP:CE2	1:B:316:LEU:HD22	2.41	0.55
1:B:174:LYS:HE3	1:B:178:ASP:OD2	2.07	0.55
1:A:55:GLY:O	1:A:56:GLY:C	2.49	0.55
1:A:52:TRP:O	1:A:72:VAL:HA	2.05	0.55
1:A:68:LYS:O	1:A:69:ASP:HB2	2.05	0.55
1:B:56:GLY:HA2	1:B:59:ARG:NH1	2.22	0.55
1:B:244:GLN:NE2	1:B:303:PRO:HB3	2.21	0.55
1:B:303:PRO:HG2	1:B:355:LEU:CD1	2.37	0.55
1:B:41:MET:CE	1:B:53:LEU:HD13	2.37	0.55
1:B:374:GLY:CA	1:B:427:LEU:HD22	2.30	0.55
1:A:82:ARG:HB2	1:A:82:ARG:HH11	1.71	0.55
1:A:365:LEU:HD12	1:A:389:ALA:HB2	1.88	0.55
1:A:52:TRP:CE3	1:A:160:SER:HB2	2.40	0.55
1:A:76:ALA:HB3	1:A:81:VAL:HG22	1.89	0.55
1:A:181:ILE:HD11	1:A:210:MET:HG3	1.88	0.55
1:A:77:THR:HB	1:A:80:GLN:HG3	1.89	0.55
1:B:50:GLU:CG	1:B:52:TRP:HE1	2.20	0.55
1:B:418:SER:O	1:B:423:GLN:NE2	2.33	0.55
1:B:74:THR:HG23	1:B:76:ALA:H	1.72	0.54
1:A:143:ILE:HD11	1:A:158:TYR:CD2	2.42	0.54
1:A:418:SER:O	1:A:423:GLN:NE2	2.40	0.54
1:A:358:LEU:HD12	1:A:358:LEU:H	1.73	0.54
1:B:153:THR:HG21	1:B:175:ASP:OD2	2.07	0.54
1:A:277:ASP:O	1:A:282:ARG:HD2	2.07	0.54
1:B:34:SER:CB	1:B:38:LEU:HD21	2.38	0.54
1:A:244:GLN:NE2	1:A:303:PRO:HA	2.21	0.54
1:B:342:LEU:HD21	1:B:363:TRP:HZ3	1.72	0.54
1:A:280:MET:HA	1:A:313:TYR:CD2	2.42	0.54
1:A:342:LEU:O	1:A:346:CYS:HB2	2.07	0.54
1:A:380:LEU:C	1:A:382:GLU:N	2.65	0.54
1:B:311:PHE:HE1	1:B:345:ALA:HB2	1.72	0.53
1:B:53:LEU:HD12	1:B:71:ASP:O	2.09	0.53
1:B:271:TYR:HB2	1:B:280:MET:HE3	1.89	0.53
1:A:18:VAL:HG13	1:A:18:VAL:O	2.09	0.53
1:B:151:ASP:HB3	1:B:152:PHE:CD2	2.44	0.53
1:A:262:GLN:CB	1:A:263:PRO:HD3	2.37	0.53
1:B:152:PHE:CZ	1:B:201:ALA:HA	2.44	0.53
1:B:183:LEU:HD12	1:B:191:TYR:CE1	2.44	0.53
1:A:72:VAL:HG22	1:A:109:VAL:HG22	1.90	0.53
1:A:216:THR:HG22	1:A:216:THR:O	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:C	1:B:92:GLY:H	2.17	0.52
1:B:278:SER:O	1:B:282:ARG:HG3	2.09	0.52
1:B:374:GLY:C	1:B:376:ARG:H	2.17	0.52
1:A:28:ILE:HG23	1:A:28:ILE:O	2.10	0.52
1:A:326:SER:O	1:A:328:LEU:N	2.42	0.52
1:B:82:ARG:HG3	1:B:82:ARG:NH1	2.24	0.52
1:B:385:LYS:HA	1:B:385:LYS:HZ3	1.74	0.52
1:A:60:ASP:HA	1:A:63:LEU:HD12	1.91	0.52
1:B:68:LYS:HE3	1:B:207:LYS:HZ2	1.74	0.52
1:B:73:THR:HA	1:B:110:ALA:O	2.09	0.52
1:B:154:ILE:HD13	1:B:210:MET:CE	2.34	0.52
1:A:196:VAL:HG21	1:A:234:ARG:CZ	2.39	0.52
1:A:270:ARG:HD2	1:A:271:TYR:CE2	2.43	0.52
1:B:170:VAL:HG11	1:B:184:ILE:HD11	1.91	0.52
1:A:402:ASN:ND2	1:A:404:GLU:N	2.58	0.52
1:B:183:LEU:CD2	1:B:184:ILE:N	2.65	0.52
1:A:402:ASN:C	1:A:402:ASN:ND2	2.66	0.52
1:B:158:TYR:O	1:B:166:VAL:HG23	2.10	0.52
1:A:103:GLY:C	1:A:105:GLU:H	2.18	0.52
1:A:249:TYR:CE1	1:A:253:LYS:HE3	2.44	0.52
1:B:150:ARG:HD3	1:B:156:SER:OG	2.10	0.52
1:A:76:ALA:HB3	1:A:81:VAL:CG2	2.39	0.52
1:A:202:VAL:CG2	1:A:254:LEU:HB3	2.40	0.52
1:A:381:LEU:HD23	1:A:415:PHE:CE2	2.45	0.52
1:B:322:ILE:HG22	1:B:333:ALA:HB1	1.91	0.52
1:B:383:HIS:ND1	1:B:384:PRO:HD2	2.24	0.52
1:A:387:ARG:HG2	1:A:387:ARG:HH11	1.75	0.51
1:B:185:GLY:H	1:B:190:ARG:NH1	2.08	0.51
1:B:302:ASN:O	1:B:305:PHE:HB3	2.10	0.51
1:B:77:THR:HG23	1:B:80:GLN:NE2	2.24	0.51
1:A:369:MET:O	1:A:408:LEU:HD12	2.10	0.51
1:B:72:VAL:CG2	1:B:109:VAL:HG22	2.41	0.51
1:A:191:TYR:HD1	1:A:198:MET:HE2	1.75	0.51
1:A:361:ASP:O	1:A:365:LEU:HG	2.11	0.51
1:A:383:HIS:ND1	1:A:384:PRO:HD2	2.25	0.51
1:B:170:VAL:CG1	1:B:171:GLY:H	2.13	0.51
1:B:419:ALA:HB1	1:B:420:PRO:HD2	1.91	0.51
1:A:97:LEU:HD21	1:A:108:GLU:OE1	2.11	0.51
1:A:390:TYR:HE2	1:B:417:VAL:O	1.93	0.51
1:A:158:TYR:O	1:A:166:VAL:HA	2.11	0.51
1:A:183:LEU:HB2	1:A:216:THR:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG23	1:A:310:MET:HG2	1.92	0.51
1:B:183:LEU:CD1	1:B:191:TYR:CE1	2.94	0.51
1:B:190:ARG:HG3	1:B:190:ARG:NH1	2.25	0.51
1:A:181:ILE:HD11	1:A:210:MET:CG	2.41	0.50
1:A:236:PHE:O	1:A:237:GLU:C	2.53	0.50
1:B:82:ARG:HH22	1:B:86:ARG:NH2	2.09	0.50
1:B:365:LEU:O	1:B:369:MET:HG3	2.11	0.50
1:A:312:TRP:CE2	1:A:396:ARG:HD2	2.46	0.50
1:A:164:PHE:N	1:A:164:PHE:CD1	2.79	0.50
1:A:283:ILE:HG22	1:A:284:ILE:N	2.26	0.50
1:B:244:GLN:NE2	1:B:303:PRO:CA	2.74	0.50
1:A:61:LEU:HD23	1:A:67:PRO:HD3	1.91	0.50
1:A:75:ASN:HD22	1:A:75:ASN:N	1.98	0.50
1:A:233:ALA:HA	1:A:350:ALA:HB3	1.94	0.50
1:B:289:LYS:O	1:B:292:ASP:HB2	2.10	0.50
1:B:28:ILE:O	1:B:29:SER:C	2.54	0.50
1:B:402:ASN:ND2	1:B:402:ASN:C	2.69	0.50
1:A:387:ARG:HG2	1:A:387:ARG:NH1	2.26	0.50
1:B:154:ILE:HG21	1:B:210:MET:HE1	1.93	0.49
1:A:59:ARG:HE	1:A:208:LEU:HD21	1.77	0.49
1:B:55:GLY:O	1:B:58:VAL:CG1	2.56	0.49
1:A:38:LEU:O	1:A:42:TYR:CD1	2.65	0.49
1:A:40:VAL:HG11	1:A:107:ILE:HG21	1.93	0.49
1:A:268:ILE:O	1:A:269:THR:C	2.56	0.49
1:A:301:VAL:HG22	1:A:302:ASN:N	2.27	0.49
1:A:170:VAL:CG1	1:A:171:GLY:N	2.74	0.49
1:B:61:LEU:CD2	1:B:67:PRO:HD3	2.43	0.49
1:A:171:GLY:O	1:A:172:GLY:C	2.54	0.49
1:A:195:PRO:O	1:A:198:MET:HE3	2.13	0.49
1:A:213:SER:HB3	1:A:216:THR:HB	1.95	0.49
1:A:372:ARG:HA	1:A:372:ARG:CZ	2.38	0.49
1:B:312:TRP:NE1	1:B:396:ARG:HD2	2.28	0.49
1:B:24:GLU:OE1	1:B:24:GLU:N	2.46	0.49
1:B:150:ARG:HH21	1:B:150:ARG:HG3	1.77	0.49
1:A:63:LEU:HD21	1:A:176:LEU:HD11	1.94	0.49
1:A:77:THR:CB	1:A:80:GLN:HG3	2.43	0.48
1:B:28:ILE:HD12	1:B:30:ARG:HH21	1.78	0.48
1:B:148:GLN:O	1:B:184:ILE:HG21	2.13	0.48
1:A:35:GLU:HG2	1:A:105:GLU:OE1	2.12	0.48
1:B:152:PHE:CD1	1:B:181:ILE:HG22	2.48	0.48
1:A:179:GLY:C	1:A:210:MET:HB2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:MET:C	1:A:102:PHE:HD1	2.21	0.48
1:B:30:ARG:CD	1:B:33:ILE:HD11	2.44	0.48
1:B:244:GLN:HE22	1:B:303:PRO:CA	2.20	0.48
1:B:367:LEU:O	1:B:370:SER:HB3	2.14	0.48
1:B:83:LYS:C	1:B:85:PHE:H	2.22	0.48
1:B:287:VAL:HG21	1:B:309:ALA:HB1	1.94	0.48
1:B:26:HIS:C	1:B:26:HIS:CD2	2.91	0.48
1:B:34:SER:C	1:B:35:GLU:O	2.56	0.48
1:A:72:VAL:CG2	1:A:109:VAL:HG22	2.43	0.47
1:A:75:ASN:ND2	1:A:75:ASN:N	2.60	0.47
1:B:56:GLY:O	1:B:59:ARG:HB3	2.14	0.47
1:B:271:TYR:HB2	1:B:280:MET:CE	2.44	0.47
1:A:38:LEU:HB3	1:A:42:TYR:CE1	2.48	0.47
1:B:34:SER:O	1:B:38:LEU:HD23	2.14	0.47
1:B:157:LEU:HD21	1:B:172:GLY:HA3	1.95	0.47
1:A:90:LEU:CD2	1:A:90:LEU:H	2.27	0.47
1:A:35:GLU:HB2	1:A:70:PHE:CE1	2.50	0.47
1:A:160:SER:HB3	1:A:163:ASP:OD1	2.14	0.47
1:A:358:LEU:O	1:A:359:THR:C	2.58	0.47
1:A:61:LEU:CD2	1:A:67:PRO:HD3	2.44	0.47
1:A:373:GLN:HG2	1:A:376:ARG:HG3	1.95	0.47
1:A:388:ALA:O	1:A:389:ALA:C	2.58	0.47
1:B:82:ARG:HH22	1:B:86:ARG:HH21	1.61	0.47
1:B:227:LEU:O	1:B:230:ILE:HB	2.14	0.47
1:B:325:GLU:C	1:B:327:GLY:N	2.66	0.47
1:B:376:ARG:O	1:B:379:LYS:HB3	2.14	0.47
1:A:154:ILE:HG22	1:A:176:LEU:HB2	1.97	0.47
1:A:303:PRO:HD2	1:A:304:ALA:H	1.78	0.47
1:A:411:TRP:C	1:A:413:GLY:N	2.70	0.47
1:B:399:VAL:HG23	1:B:400:GLU:N	2.29	0.47
1:A:273:THR:C	1:A:275:ASN:N	2.71	0.47
1:A:76:ALA:O	1:A:77:THR:C	2.58	0.47
1:A:374:GLY:C	1:A:376:ARG:H	2.22	0.47
1:B:26:HIS:HD2	1:B:27:ALA:O	1.97	0.47
1:A:22:PRO:HG2	1:A:25:GLN:NE2	2.29	0.46
1:B:90:LEU:HA	1:B:99:HIS:O	2.15	0.46
1:B:153:THR:HG22	1:B:170:VAL:HG12	1.97	0.46
1:B:311:PHE:H	1:B:311:PHE:HD2	1.63	0.46
1:A:334:PHE:C	1:A:334:PHE:CD2	2.93	0.46
1:A:374:GLY:CA	1:A:427:LEU:HD22	2.42	0.46
1:B:261:PHE:CE2	1:B:265:PHE:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LEU:O	1:B:289:LYS:C	2.59	0.46
1:B:356:THR:O	1:B:360:ARG:HG2	2.15	0.46
1:A:273:THR:HG23	1:A:278:SER:HB2	1.97	0.46
1:B:26:HIS:CD2	1:B:26:HIS:O	2.68	0.46
1:A:95:PHE:CE1	1:A:96:ARG:NE	2.80	0.46
1:A:370:SER:HA	1:A:408:LEU:CD1	2.46	0.46
1:B:392:LEU:HD12	1:B:392:LEU:O	2.16	0.46
1:B:358:LEU:HB3	1:B:385:LYS:HD2	1.98	0.46
1:A:235:LEU:O	1:A:239:SER:HB3	2.15	0.46
1:A:20:VAL:O	1:A:20:VAL:HG13	2.16	0.46
1:A:270:ARG:HD2	1:A:271:TYR:HE2	1.81	0.46
1:B:411:TRP:C	1:B:413:GLY:N	2.74	0.46
1:A:304:ALA:HB2	1:A:355:LEU:HD12	1.98	0.46
1:B:30:ARG:NH2	1:B:33:ILE:HD11	2.30	0.46
1:B:400:GLU:C	1:B:402:ASN:H	2.24	0.46
1:A:37:ALA:O	1:A:40:VAL:CG1	2.53	0.45
1:B:278:SER:CB	1:B:279:PRO:CD	2.93	0.45
1:A:26:HIS:CD2	1:A:26:HIS:C	2.94	0.45
1:A:152:PHE:CZ	1:A:201:ALA:HA	2.52	0.45
1:A:385:LYS:O	1:A:386:PHE:C	2.59	0.45
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.76	0.45
1:A:234:ARG:C	1:A:236:PHE:N	2.72	0.45
1:A:283:ILE:CG2	1:A:284:ILE:N	2.80	0.45
1:B:23:ARG:HB3	1:B:164:PHE:O	2.17	0.45
1:B:97:LEU:HD11	1:B:108:GLU:CG	2.45	0.45
1:B:208:LEU:HD12	1:B:208:LEU:H	1.81	0.45
1:A:186:ASN:O	1:A:187:PRO:C	2.58	0.45
1:B:55:GLY:C	1:B:58:VAL:HG12	2.41	0.45
1:B:311:PHE:C	1:B:314:PRO:HD2	2.42	0.45
1:B:325:GLU:HG2	1:B:326:SER:N	2.31	0.45
1:A:21:ILE:HG13	1:A:25:GLN:HG3	1.99	0.45
1:A:170:VAL:CG1	1:A:171:GLY:H	2.30	0.45
1:A:219:PRO:O	1:A:223:LEU:HD12	2.17	0.45
1:A:220:ILE:HG23	1:A:260:LEU:HD11	1.99	0.45
1:B:41:MET:HE2	1:B:53:LEU:HD13	1.98	0.45
1:B:244:GLN:NE2	1:B:303:PRO:CB	2.79	0.45
1:B:85:PHE:C	1:B:87:ASN:N	2.74	0.45
1:B:175:ASP:OD2	1:B:182:ARG:NH1	2.49	0.45
1:A:47:ALA:CB	1:A:84:LEU:HD21	2.47	0.45
1:A:77:THR:HB	1:A:80:GLN:H	1.82	0.45
1:A:385:LYS:HA	1:A:385:LYS:HD3	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PRO:CG	1:B:70:PHE:CZ	3.00	0.45
1:A:400:GLU:O	1:A:401:ARG:C	2.60	0.45
1:B:91:VAL:O	1:B:92:GLY:O	2.34	0.45
1:A:34:SER:O	1:A:35:GLU:C	2.61	0.44
1:A:273:THR:O	1:A:274:GLU:C	2.60	0.44
1:B:90:LEU:C	1:B:92:GLY:N	2.74	0.44
1:A:151:ASP:HB3	1:A:152:PHE:CD2	2.53	0.44
1:A:264:LEU:C	1:A:266:PRO:HD3	2.42	0.44
1:B:36:ASN:O	1:B:102:PHE:CE1	2.71	0.44
1:B:280:MET:O	1:B:284:ILE:HG13	2.17	0.44
1:A:27:ALA:O	1:A:28:ILE:C	2.60	0.44
1:A:112:PHE:O	1:A:140:PHE:HB3	2.18	0.44
1:B:323:ALA:C	1:B:325:GLU:H	2.26	0.44
1:A:380:LEU:O	1:A:382:GLU:N	2.50	0.44
1:B:144:GLU:HA	1:B:169:TYR:CE1	2.53	0.44
1:A:20:VAL:HG23	1:A:167:ARG:HD3	1.99	0.44
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.87	0.44
1:A:363:TRP:O	1:A:364:GLN:C	2.60	0.44
1:B:37:ALA:HB2	1:B:107:ILE:HG12	1.99	0.44
1:B:164:PHE:CD1	1:B:164:PHE:N	2.85	0.44
1:B:311:PHE:CD2	1:B:311:PHE:N	2.86	0.44
1:A:42:TYR:HB3	1:A:46:LYS:NZ	2.32	0.44
1:A:91:VAL:O	1:A:92:GLY:O	2.35	0.44
1:A:198:MET:HE3	1:A:198:MET:HB2	1.68	0.44
1:A:218:GLU:HB3	1:A:219:PRO:CD	2.40	0.44
1:A:143:ILE:HD11	1:A:158:TYR:CG	2.52	0.44
1:A:148:GLN:O	1:A:184:ILE:HG21	2.18	0.44
1:A:283:ILE:HG13	1:A:313:TYR:HE2	1.83	0.44
1:A:380:LEU:C	1:A:382:GLU:H	2.26	0.44
1:B:338:MET:O	1:B:342:LEU:HD22	2.18	0.44
1:B:152:PHE:CD2	1:B:152:PHE:N	2.86	0.44
1:B:158:TYR:CD1	1:B:158:TYR:N	2.86	0.44
1:B:290:ASN:C	1:B:292:ASP:N	2.72	0.44
1:B:305:PHE:O	1:B:306:LEU:C	2.61	0.44
1:B:168:ASP:OD1	1:B:170:VAL:O	2.35	0.43
1:B:307:PHE:C	1:B:309:ALA:N	2.76	0.43
1:B:202:VAL:O	1:B:205:ALA:HB3	2.19	0.43
1:A:52:TRP:HB2	1:A:73:THR:HG23	2.00	0.43
1:B:153:THR:HG22	1:B:170:VAL:CG1	2.48	0.43
1:B:352:PRO:O	1:B:353:LYS:C	2.59	0.43
1:A:77:THR:O	1:A:81:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:NH2	1:A:416:GLN:HE22	2.16	0.43
1:A:421:PRO:O	1:A:424:LYS:HB2	2.18	0.43
1:B:93:ARG:HG2	1:B:94:ARG:H	1.83	0.43
1:A:202:VAL:HG11	1:A:255:LEU:CD2	2.48	0.43
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.85	0.43
1:B:96:ARG:HG3	1:B:97:LEU:H	1.84	0.43
1:B:414:GLU:CB	1:B:426:MET:HE1	2.48	0.43
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.82	0.43
1:A:194:ASP:OD2	1:A:196:VAL:HG23	2.18	0.43
1:B:72:VAL:HG23	1:B:109:VAL:HA	2.01	0.43
1:B:227:LEU:HD11	1:B:260:LEU:HD22	2.01	0.43
1:B:311:PHE:CE1	1:B:345:ALA:HB1	2.54	0.43
1:B:411:TRP:O	1:B:414:GLU:N	2.51	0.43
1:A:45:ASN:C	1:A:47:ALA:N	2.74	0.43
1:B:268:ILE:O	1:B:269:THR:C	2.60	0.43
1:B:150:ARG:O	1:B:184:ILE:CG1	2.66	0.43
1:B:184:ILE:HB	1:B:190:ARG:HH12	1.83	0.43
1:A:93:ARG:O	1:A:94:ARG:O	2.37	0.43
1:A:266:PRO:O	1:A:268:ILE:N	2.52	0.43
1:B:251:THR:O	1:B:255:LEU:HG	2.18	0.43
1:B:26:HIS:O	1:B:27:ALA:C	2.62	0.42
1:B:167:ARG:HG2	1:B:167:ARG:NH1	2.33	0.42
1:B:400:GLU:C	1:B:402:ASN:N	2.77	0.42
1:A:191:TYR:HE1	1:A:198:MET:HG3	1.78	0.42
1:A:387:ARG:HH22	1:A:416:GLN:HE22	1.65	0.42
1:B:53:LEU:O	1:B:58:VAL:HG21	2.19	0.42
1:B:235:LEU:O	1:B:236:PHE:C	2.62	0.42
1:A:415:PHE:O	1:A:415:PHE:CG	2.72	0.42
1:A:358:LEU:HD23	1:A:385:LYS:CE	2.49	0.42
1:A:413:GLY:O	1:A:417:VAL:HG22	2.20	0.42
1:A:30:ARG:HD2	1:A:33:ILE:HD11	2.01	0.42
1:A:41:MET:O	1:A:44:LEU:HB2	2.19	0.42
1:A:369:MET:HE1	1:A:390:TYR:HA	2.01	0.42
1:B:33:ILE:O	1:B:33:ILE:HG22	2.19	0.42
1:B:102:PHE:HB2	1:B:105:GLU:O	2.19	0.42
1:B:311:PHE:HE1	1:B:345:ALA:HB1	1.80	0.42
1:A:95:PHE:O	1:A:96:ARG:HB2	2.20	0.42
1:A:267:THR:HG21	1:A:341:VAL:HG13	2.00	0.42
1:A:363:TRP:O	1:A:366:GLN:HB2	2.20	0.42
1:A:408:LEU:O	1:A:412:TRP:HD1	2.03	0.42
1:B:287:VAL:HG11	1:B:306:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:TRP:CE2	1:B:396:ARG:HD2	2.54	0.42
1:B:407:ARG:HG2	1:B:407:ARG:NH1	2.34	0.42
1:B:411:TRP:O	1:B:412:TRP:C	2.62	0.42
1:B:291:THR:O	1:B:295:ILE:HG12	2.19	0.42
1:A:273:THR:OG1	1:A:275:ASN:HB3	2.20	0.42
1:B:415:PHE:O	1:B:415:PHE:CG	2.72	0.42
1:A:374:GLY:O	1:A:376:ARG:N	2.52	0.42
1:A:402:ASN:HD21	1:A:404:GLU:HB3	1.84	0.42
1:B:199:LEU:O	1:B:202:VAL:HG23	2.20	0.42
1:B:362:ILE:O	1:B:366:GLN:HG2	2.19	0.42
1:B:372:ARG:HB2	1:B:372:ARG:HH11	1.85	0.42
1:B:418:SER:O	1:B:423:GLN:HG3	2.20	0.42
1:A:26:HIS:O	1:A:26:HIS:HD2	2.02	0.41
1:A:82:ARG:NH1	1:A:82:ARG:CB	2.74	0.41
1:A:152:PHE:CE1	1:A:201:ALA:HA	2.55	0.41
1:A:334:PHE:C	1:A:334:PHE:HD2	2.27	0.41
1:A:367:LEU:O	1:A:368:ARG:C	2.63	0.41
1:B:30:ARG:HD3	1:B:33:ILE:HD11	2.01	0.41
1:B:402:ASN:HD22	1:B:403:ALA:N	2.17	0.41
1:A:355:LEU:N	1:A:355:LEU:HD22	2.36	0.41
1:B:218:GLU:CB	1:B:219:PRO:HD3	2.43	0.41
1:B:303:PRO:CG	1:B:355:LEU:HD11	2.47	0.41
1:B:370:SER:HA	1:B:408:LEU:HD11	2.02	0.41
1:A:28:ILE:O	1:A:30:ARG:HG2	2.20	0.41
1:B:96:ARG:CG	1:B:97:LEU:N	2.83	0.41
1:B:113:ARG:HD3	1:B:146:ASP:OD1	2.20	0.41
1:B:148:GLN:C	1:B:150:ARG:H	2.27	0.41
1:B:236:PHE:CE2	1:B:351:ILE:HG12	2.56	0.41
1:A:158:TYR:CD1	1:A:158:TYR:N	2.89	0.41
1:A:58:VAL:O	1:A:62:LEU:HD12	2.21	0.41
1:A:302:ASN:HB3	1:A:305:PHE:HB2	2.02	0.41
1:B:358:LEU:N	1:B:358:LEU:HD12	2.35	0.41
1:A:97:LEU:HD22	1:A:108:GLU:HG2	2.03	0.41
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.93	0.41
1:A:212:ILE:HD13	1:A:258:TYR:OH	2.19	0.41
1:A:358:LEU:H	1:A:358:LEU:CD1	2.33	0.41
1:A:220:ILE:O	1:A:221:PRO:C	2.64	0.41
1:A:351:ILE:HA	1:A:352:PRO:HD3	1.92	0.41
1:B:279:PRO:CD	1:B:280:MET:H	2.34	0.41
1:A:23:ARG:HA	1:A:26:HIS:CE1	2.56	0.41
1:A:42:TYR:O	1:A:46:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:SER:O	1:A:327:GLY:C	2.63	0.41
1:A:395:LEU:O	1:A:398:GLU:N	2.53	0.41
1:B:21:ILE:HB	1:B:166:VAL:HG12	2.02	0.41
1:B:313:TYR:N	1:B:314:PRO:CD	2.84	0.41
1:B:352:PRO:HG3	1:B:355:LEU:HD23	2.03	0.41
1:B:411:TRP:O	1:B:413:GLY:N	2.54	0.41
1:A:405:LEU:C	1:A:407:ARG:H	2.28	0.41
1:B:49:TYR:CE1	1:B:80:GLN:OE1	2.74	0.41
1:B:231:PRO:HA	1:B:232:PRO:HD3	1.89	0.41
1:B:158:TYR:N	1:B:158:TYR:HD1	2.19	0.40
1:B:215:GLU:CD	1:B:215:GLU:H	2.28	0.40
1:A:90:LEU:H	1:A:90:LEU:HD23	1.85	0.40
1:A:173:MET:O	1:A:174:LYS:C	2.65	0.40
1:A:184:ILE:CG2	1:A:190:ARG:HH12	2.21	0.40
1:A:391:ASP:O	1:A:395:LEU:HD13	2.21	0.40
1:B:49:TYR:CD1	1:B:76:ALA:HB2	2.55	0.40
1:B:61:LEU:HD21	1:B:67:PRO:HD3	2.03	0.40
1:B:170:VAL:CG1	1:B:171:GLY:N	2.75	0.40
1:A:152:PHE:CD2	1:A:152:PHE:N	2.88	0.40
1:B:59:ARG:HD2	1:B:154:ILE:HD12	2.04	0.40
1:B:395:LEU:O	1:B:396:ARG:C	2.64	0.40
1:A:20:VAL:HG23	1:A:167:ARG:HE	1.84	0.40
1:A:262:GLN:NE2	1:A:269:THR:HG21	2.36	0.40
1:B:55:GLY:N	1:B:58:VAL:HG11	2.36	0.40
1:B:64:GLY:O	1:B:65:LYS:O	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH1	1:A:361:ASP:OD1[2_545]	1.75	0.45

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	384/415 (92%)	291 (76%)	72 (19%)	21 (6%)	1	9
1	B	384/415 (92%)	298 (78%)	57 (15%)	29 (8%)	1	4
All	All	768/830 (92%)	589 (77%)	129 (17%)	50 (6%)	1	6

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	92	GLY
1	A	245	ALA
1	A	372	ARG
1	A	375	LYS
1	B	28	ILE
1	B	35	GLU
1	B	65	LYS
1	B	92	GLY
1	B	104	PRO
1	B	105	GLU
1	B	278	SER
1	B	298	ASP
1	A	27	ALA
1	A	56	GLY
1	A	65	LYS
1	A	69	ASP
1	A	94	ARG
1	A	139	ILE
1	A	172	GLY
1	A	267	THR
1	A	327	GLY
1	A	401	ARG
1	B	27	ALA
1	B	56	GLY
1	B	97	LEU
1	B	151	ASP
1	B	172	GLY
1	B	311	PHE
1	B	327	GLY
1	A	31	LYS
1	A	369	MET
1	B	225	THR

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Mol	Chain	Res	Type
1	B	244	GLN
1	B	299	MET
1	A	244	GLN
1	B	88	CYS
1	B	185	GLY
1	B	207	LYS
1	B	401	ARG
1	B	91	VAL
1	B	93	ARG
1	B	324	GLN
1	A	184	ILE
1	A	415	PHE
1	B	31	LYS
1	B	84	LEU
1	B	248	GLY
1	B	279	PRO
1	A	187	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/358 (93%)	284 (85%)	50 (15%)	3	13
1	B	334/358 (93%)	277 (83%)	57 (17%)	2	9
All	All	668/716 (93%)	561 (84%)	107 (16%)	2	11

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	29	SER
1	A	30	ARG
1	A	36	ASN
1	A	38	LEU
1	A	72	VAL

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Mol	Chain	Res	Type
1	A	73	THR
1	A	75	ASN
1	A	84	LEU
1	A	89	ARG
1	A	90	LEU
1	A	100	VAL
1	A	143	ILE
1	A	149	ARG
1	A	150	ARG
1	A	161	VAL
1	A	164	PHE
1	A	166	VAL
1	A	184	ILE
1	A	198	MET
1	A	208	LEU
1	A	210	MET
1	A	212	ILE
1	A	215	GLU
1	A	225	THR
1	A	226	LEU
1	A	244	GLN
1	A	256	CYS
1	A	277	ASP
1	A	280	MET
1	A	283	ILE
1	A	291	THR
1	A	328	LEU
1	A	334	PHE
1	A	336	LEU
1	A	343	ASP
1	A	344	GLU
1	A	346	CYS
1	A	348	SER
1	A	349	LEU
1	A	357	THR
1	A	364	GLN
1	A	368	ARG
1	A	375	LYS
1	A	381	LEU
1	A	387	ARG
1	A	402	ASN
1	A	404	GLU

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Mol	Chain	Res	Type
1	A	408	LEU
1	A	420	PRO
1	B	21	ILE
1	B	24	GLU
1	B	26	HIS
1	B	30	ARG
1	B	38	LEU
1	B	82	ARG
1	B	100	VAL
1	B	104	PRO
1	B	106	ILE
1	B	108	GLU
1	B	139	ILE
1	B	142	SER
1	B	148	GLN
1	B	167	ARG
1	B	189	THR
1	B	202	VAL
1	B	208	LEU
1	B	215	GLU
1	B	216	THR
1	B	220	ILE
1	B	225	THR
1	B	226	LEU
1	B	244	GLN
1	B	256	CYS
1	B	267	THR
1	B	269	THR
1	B	275	ASN
1	B	277	ASP
1	B	280	MET
1	B	282	ARG
1	B	283	ILE
1	B	287	VAL
1	B	291	THR
1	B	296	HIS
1	B	298	ASP
1	B	300	ARG
1	B	302	ASN
1	B	316	LEU
1	B	324	GLN
1	B	325	GLU

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Mol	Chain	Res	Type
1	B	326	SER
1	B	329	THR
1	B	342	LEU
1	B	343	ASP
1	B	346	CYS
1	B	348	SER
1	B	349	LEU
1	B	354	ARG
1	B	371	ARG
1	B	372	ARG
1	B	385	LYS
1	B	401	ARG
1	B	405	LEU
1	B	406	GLN
1	B	407	ARG
1	B	408	LEU
1	B	420	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	26	HIS
1	A	36	ASN
1	A	45	ASN
1	A	75	ASN
1	A	80	GLN
1	A	87	ASN
1	A	138	ASN
1	A	155	ASN
1	A	244	GLN
1	A	262	GLN
1	A	275	ASN
1	A	290	ASN
1	A	302	ASN
1	A	364	GLN
1	A	402	ASN
1	A	406	GLN
1	A	416	GLN
1	A	423	GLN
1	B	26	HIS
1	B	36	ASN

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Mol	Chain	Res	Type
1	B	45	ASN
1	B	87	ASN
1	B	155	ASN
1	B	186	ASN
1	B	244	GLN
1	B	275	ASN
1	B	290	ASN
1	B	364	GLN
1	B	373	GLN
1	B	402	ASN
1	B	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	388/415 (93%)	0.32	15 (3%)	43 25	71, 101, 141, 169	0
1	B	388/415 (93%)	0.25	11 (2%)	55 34	66, 104, 145, 166	0
All	All	776/830 (93%)	0.29	26 (3%)	48 28	66, 103, 143, 169	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	ILE	3.8
1	A	409	VAL	3.8
1	A	399	VAL	3.0
1	A	377	ALA	2.9
1	A	392	LEU	2.8
1	A	311	PHE	2.8
1	B	311	PHE	2.6
1	A	35	GLU	2.6
1	A	91	VAL	2.6
1	B	377	ALA	2.4
1	B	139	ILE	2.4
1	B	350	ALA	2.4
1	A	369	MET	2.4
1	A	333	ALA	2.3
1	A	75	ASN	2.2
1	B	345	ALA	2.2
1	B	291	THR	2.2
1	B	412	TRP	2.2
1	A	28	ILE	2.2
1	A	408	LEU	2.1
1	A	406	GLN	2.1
1	A	309	ALA	2.1
1	B	334	PHE	2.1
1	B	114	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	105	GLU	2.0
1	B	392	LEU	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](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	501	1/1	0.87	0.20	37,37,37,37	0
2	MG	B	501	1/1	0.92	0.12	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.