



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 3FPP / pdb_00003fpp
Title : Crystal structure of E.coli MacA
Authors : Yum, S.; Xu, Y.; Piao, S.; Ha, N.-C.
Deposited on : 2009-01-06
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

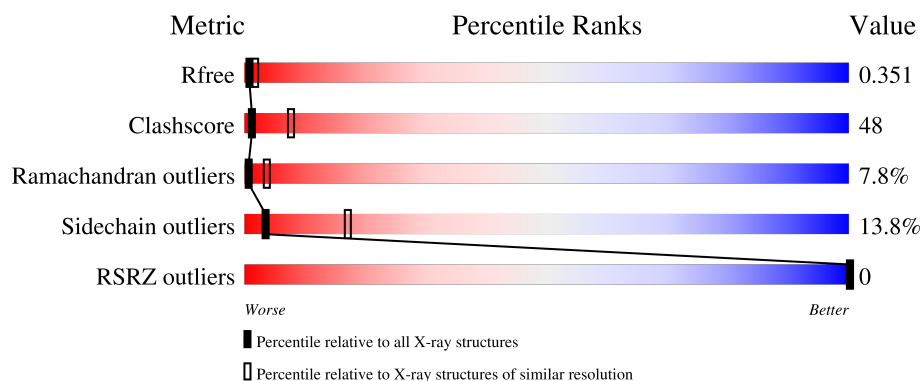
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

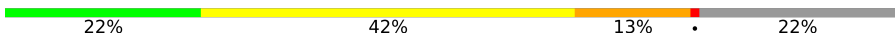
The reported resolution of this entry is 2.99 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	341	
1	B	341	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4097 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 Macrolide-specific efflux protein macA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2043	1274	361	402	6			
1	B	267	Total	C	N	O	S	0	0	0
			2054	1280	365	403	6			

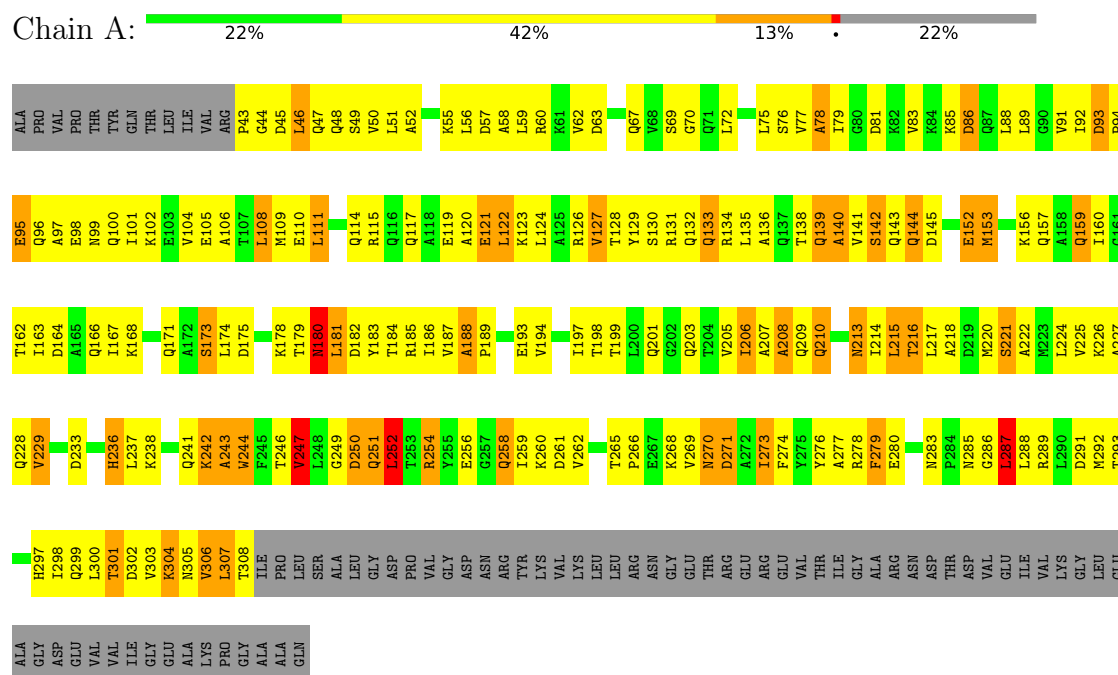
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	GLN	LYS	SEE REMARK 999	UNP P75830
A	148	ASN	THR	SEE REMARK 999	UNP P75830
A	251	GLN	PRO	SEE REMARK 999	UNP P75830
B	139	GLN	LYS	SEE REMARK 999	UNP P75830
B	148	ASN	THR	SEE REMARK 999	UNP P75830
B	251	GLN	PRO	SEE REMARK 999	UNP P75830

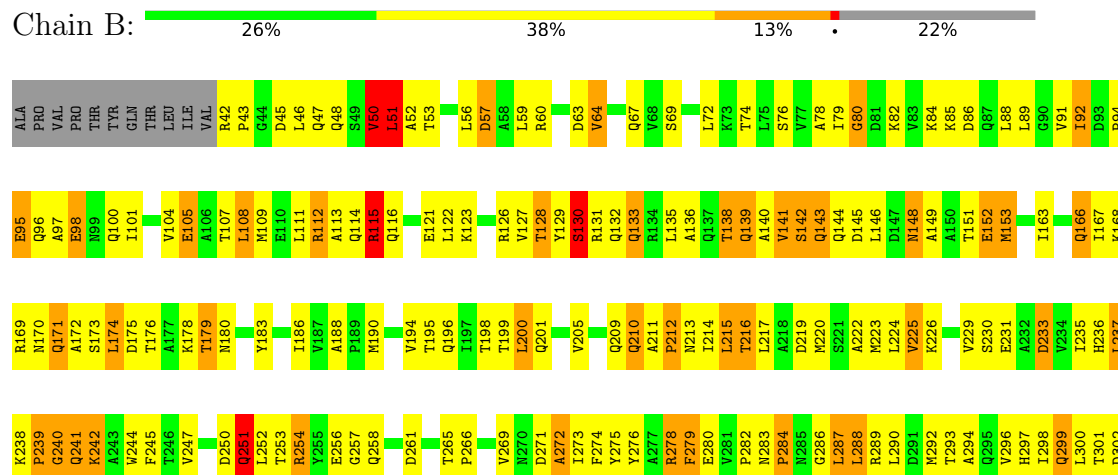
3 Residue-property plots

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: Macrolide-specific efflux protein macA



- Molecule 1: Macrolide-specific efflux protein macA



GLY	V303
GLU	K304
ALA	N305
LYS	V306
PRO	L307
GLY	T308
ALA	ILE
ALA	PRO
GLN	LEU
	SER
	ALA
	LEU
	GLY
	ASP
	ASN
	ARG
	TYR
	LYS
	VAL
	LYS
	LEU
	LEU
	ARG
	ASN
	GLY
	GLU
	THR
	ARG
	GLU
	ARG
	GLU
	VAL
	THR
	ILE
	GLY
	ALA
	ARG
	ASN
	ASP
	THR
	ASP
	VAL
	GLU
	ILE
	VAL
	LYS
	GLY
	LEU
	GLU
	ALA
	GLY
	ASP
	GLU
	VAL
	VAL
	ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.52Å 128.52Å 110.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.69 – 2.99 49.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (49.69-2.99) 92.1 (49.69-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.283 , 0.349 0.284 , 0.351	Depositor DCC
R_{free} test set	1950 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 12.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.447 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4097	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/2063	1.19	24/2797 (0.9%)
1	B	0.58	0/2074	1.14	20/2812 (0.7%)
All	All	0.58	0/4137	1.16	44/5609 (0.8%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	SER	N-CA-C	10.00	125.30	113.20
1	A	152	GLU	N-CA-C	-9.28	101.11	111.14
1	A	127	VAL	N-CA-C	-9.04	103.04	111.45
1	B	278	ARG	N-CA-C	8.78	121.86	110.53
1	B	143	GLN	N-CA-C	-8.03	104.08	114.04
1	A	182	ASP	N-CA-C	-8.02	103.21	113.16
1	A	283	ASN	CA-C-N	7.86	127.52	119.19
1	A	283	ASN	C-N-CA	7.86	127.52	119.19
1	A	121	GLU	N-CA-C	-7.79	102.74	111.07
1	A	173	SER	N-CA-C	-7.65	104.09	113.50
1	A	133	GLN	N-CA-C	-7.60	102.97	111.71
1	A	181	LEU	N-CA-C	-7.58	104.00	113.18
1	B	105	GLU	N-CA-C	-7.57	102.97	111.07
1	B	115	ARG	N-CA-C	-7.22	104.10	113.12
1	A	180	ASN	N-CA-C	-7.14	104.69	113.41
1	A	171	GLN	N-CA-C	-7.04	103.65	111.82
1	A	117	GLN	N-CA-C	-6.82	105.24	113.97
1	B	57	ASP	N-CA-C	6.73	118.43	108.60
1	A	93	ASP	CA-C-N	6.62	126.07	118.85
1	A	93	ASP	C-N-CA	6.62	126.07	118.85
1	A	78	ALA	N-CA-C	-6.56	99.43	109.41
1	B	64	VAL	N-CA-C	6.48	117.45	107.99
1	B	133	GLN	N-CA-C	-6.46	104.09	112.23
1	B	171	GLN	N-CA-C	-6.30	104.85	112.54
1	A	273	ILE	N-CA-C	6.28	117.15	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ALA	N-CA-C	6.27	118.73	110.08
1	B	82	LYS	N-CA-C	-6.13	101.41	110.48
1	A	120	ALA	N-CA-C	-6.07	104.02	112.45
1	B	121	GLU	N-CA-C	-6.05	104.76	111.36
1	A	236	HIS	N-CA-C	-5.97	106.15	113.50
1	B	138	THR	N-CA-C	-5.94	106.08	113.38
1	B	256	GLU	N-CA-C	5.92	117.53	108.42
1	B	173	SER	N-CA-C	-5.52	105.27	112.23
1	A	109	MET	N-CA-C	-5.51	106.73	113.50
1	B	84	LYS	N-CA-C	-5.48	101.65	110.14
1	B	233	ASP	N-CA-C	-5.31	107.46	114.04
1	A	75	LEU	N-CA-C	-5.30	100.77	109.40
1	B	153	MET	N-CA-C	-5.29	106.78	113.18
1	B	51	LEU	N-CA-C	-5.23	103.78	110.53
1	A	99	ASN	N-CA-C	-5.18	105.75	111.71
1	A	67	GLN	N-CA-C	-5.12	106.44	113.30
1	B	142	SER	CB-CA-C	-5.12	109.13	115.89
1	A	304	LYS	N-CA-C	5.08	117.77	109.59
1	B	98	GLU	N-CA-C	-5.06	105.85	111.36

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	2043	0	2104	212	0
1	B	2054	0	2116	198	0
All	All	4097	0	4220	396	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLN:HE21	1:A:159:GLN:HA	1.15	1.10
1:B:135:LEU:HD22	1:B:140:ALA:HB2	1.35	1.06
1:B:205:VAL:HG21	1:B:212:PRO:HG3	1.32	1.05
1:B:226:LYS:HZ2	1:B:278:ARG:HD3	1.23	1.04
1:A:285:ASN:ND2	1:A:286:GLY:H	1.55	1.03
1:A:242:LYS:H	1:A:242:LYS:HD2	1.20	1.02
1:B:226:LYS:NZ	1:B:278:ARG:HD3	1.74	1.00
1:A:164:ASP:O	1:A:168:LYS:HD3	1.62	0.99
1:A:124:LEU:HD21	1:B:148:ASN:ND2	1.79	0.98
1:B:109:MET:HA	1:B:112:ARG:HB2	1.50	0.93
1:B:237:LEU:HA	1:B:241:GLN:HE22	1.28	0.93
1:A:44:GLY:H	1:A:307:LEU:HA	1.30	0.93
1:A:285:ASN:CG	1:A:286:GLY:H	1.76	0.93
1:A:50:VAL:HB	1:A:298:ILE:HD11	1.50	0.92
1:A:261:ASP:HB3	1:A:278:ARG:HB2	1.49	0.92
1:B:136:ALA:HB2	1:B:146:LEU:HD21	1.52	0.92
1:A:258:GLN:H	1:A:258:GLN:NE2	1.68	0.92
1:A:243:ALA:HA	1:A:297:HIS:O	1.70	0.91
1:B:224:LEU:HD13	1:B:278:ARG:HD2	1.51	0.91
1:B:215:LEU:O	1:B:215:LEU:HD22	1.75	0.86
1:A:242:LYS:HD3	1:A:299:GLN:HB2	1.58	0.85
1:A:268:LYS:HE2	1:A:271:ASP:HA	1.56	0.85
1:B:251:GLN:HA	1:B:251:GLN:HE21	1.41	0.84
1:A:48:GLN:H	1:A:301:THR:HG23	1.42	0.84
1:B:198:THR:HB	1:B:213:ASN:HD22	1.42	0.83
1:A:242:LYS:H	1:A:242:LYS:CD	1.86	0.83
1:A:124:LEU:HD21	1:B:148:ASN:HD22	1.42	0.82
1:B:205:VAL:HG21	1:B:212:PRO:CG	2.09	0.81
1:A:285:ASN:ND2	1:A:286:GLY:N	2.29	0.81
1:A:70:GLY:HA2	1:B:67:GLN:CD	2.06	0.80
1:A:159:GLN:HA	1:A:159:GLN:NE2	1.95	0.79
1:B:56:LEU:HD13	1:B:225:VAL:HG12	1.67	0.77
1:B:136:ALA:HB1	1:B:146:LEU:HD11	1.68	0.76
1:B:224:LEU:CD1	1:B:278:ARG:HD2	2.16	0.76
1:B:74:THR:HA	1:B:201:GLN:NE2	2.02	0.75
1:B:269:VAL:HG23	1:B:269:VAL:O	1.85	0.75
1:B:59:LEU:HD22	1:B:222:ALA:HB3	1.67	0.75
1:A:105:GLU:HG2	1:A:174:LEU:HD11	1.68	0.74
1:A:159:GLN:HE21	1:A:159:GLN:CA	1.96	0.74
1:B:46:LEU:HD13	1:B:47:GLN:N	2.02	0.74
1:A:288:LEU:HA	1:A:292:MET:SD	2.28	0.74
1:A:285:ASN:CG	1:A:286:GLY:N	2.44	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PRO:HB3	1:A:305:ASN:HD21	1.52	0.74
1:B:46:LEU:HD22	1:B:47:GLN:H	1.51	0.74
1:B:92:ILE:O	1:B:94:PRO:HD3	1.88	0.73
1:A:135:LEU:HB3	1:A:140:ALA:HB3	1.68	0.73
1:A:44:GLY:H	1:A:307:LEU:CA	2.00	0.72
1:A:199:THR:HB	1:A:214:ILE:HA	1.70	0.72
1:B:56:LEU:HG	1:B:223:MET:HE3	1.69	0.72
1:B:47:GLN:HB2	1:B:301:THR:O	1.88	0.72
1:A:43:PRO:HB3	1:A:305:ASN:ND2	2.05	0.71
1:A:89:LEU:HD21	1:A:188:ALA:HB2	1.72	0.71
1:B:225:VAL:HG22	1:B:279:PHE:HB2	1.71	0.71
1:B:132:GLN:O	1:B:136:ALA:HB2	1.90	0.71
1:A:111:LEU:HA	1:A:114:GLN:HG3	1.72	0.70
1:A:47:GLN:HB2	1:A:301:THR:O	1.92	0.70
1:A:305:ASN:C	1:A:305:ASN:HD22	2.00	0.70
1:B:238:LYS:HG3	1:B:239:PRO:HD2	1.72	0.70
1:A:162:THR:HG22	1:A:166:GLN:NE2	2.07	0.69
1:B:74:THR:CG2	1:B:91:VAL:HB	2.22	0.69
1:A:126:ARG:HB3	1:A:153:MET:HE3	1.74	0.69
1:A:134:ARG:C	1:A:136:ALA:H	2.00	0.68
1:A:270:ASN:O	1:A:271:ASP:HB2	1.92	0.68
1:B:48:GLN:HG3	1:B:300:LEU:HD12	1.76	0.67
1:B:100:GLN:O	1:B:104:VAL:HG23	1.93	0.67
1:B:56:LEU:HD21	1:B:288:LEU:HB3	1.76	0.67
1:B:141:VAL:HB	1:B:145:ASP:OD2	1.95	0.67
1:B:237:LEU:HD11	1:B:298:ILE:HG21	1.77	0.67
1:A:229:VAL:HG21	1:A:237:LEU:HD22	1.77	0.67
1:B:198:THR:CB	1:B:213:ASN:HD22	2.08	0.67
1:B:48:GLN:O	1:B:300:LEU:HB2	1.95	0.66
1:A:249:GLY:O	1:A:250:ASP:HB3	1.96	0.66
1:B:247:VAL:CG2	1:B:250:ASP:HB2	2.26	0.66
1:A:238:LYS:O	1:A:241:GLN:HG3	1.96	0.66
1:B:226:LYS:HB3	1:B:276:TYR:CD2	2.31	0.65
1:A:69:SER:OG	1:A:206:ILE:HA	1.96	0.65
1:B:138:THR:O	1:B:139:GLN:HB2	1.94	0.65
1:A:268:LYS:CE	1:A:271:ASP:HA	2.26	0.65
1:B:56:LEU:CD1	1:B:225:VAL:HG12	2.26	0.65
1:A:131:ARG:O	1:A:135:LEU:HG	1.96	0.64
1:B:168:LYS:HD3	1:B:168:LYS:C	2.21	0.64
1:A:110:GLU:O	1:A:114:GLN:HG2	1.98	0.64
1:B:286:GLY:O	1:B:287:LEU:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PRO:HA	1:A:307:LEU:HB2	1.80	0.64
1:A:259:ILE:HA	1:A:279:PHE:HB3	1.79	0.63
1:A:236:HIS:HB3	1:A:300:LEU:HD13	1.80	0.63
1:A:260:LYS:NZ	1:A:280:GLU:HB2	2.13	0.63
1:B:251:GLN:HE21	1:B:251:GLN:CA	2.08	0.63
1:A:50:VAL:O	1:A:298:ILE:HG12	1.99	0.63
1:B:97:ALA:HA	1:B:100:GLN:NE2	2.13	0.63
1:B:205:VAL:CG2	1:B:212:PRO:HG3	2.20	0.63
1:B:63:ASP:OD1	1:B:216:THR:HB	1.99	0.63
1:B:283:ASN:OD1	1:B:287:LEU:O	2.17	0.62
1:A:242:LYS:CD	1:A:299:GLN:HB2	2.27	0.62
1:A:287:LEU:HD13	1:A:287:LEU:H	1.65	0.62
1:A:122:LEU:O	1:A:126:ARG:HG2	1.99	0.62
1:B:180:ASN:HA	1:B:183:TYR:HD2	1.64	0.62
1:B:226:LYS:HZ3	1:B:278:ARG:HD3	1.64	0.62
1:A:48:GLN:N	1:A:301:THR:HG23	2.13	0.61
1:A:62:VAL:HG11	1:A:189:PRO:HG3	1.82	0.60
1:B:51:LEU:HD22	1:B:297:HIS:CD2	2.36	0.60
1:A:69:SER:HA	1:A:205:VAL:O	2.01	0.60
1:B:107:THR:HG21	1:B:170:ASN:ND2	2.16	0.60
1:B:251:GLN:HA	1:B:251:GLN:NE2	2.15	0.60
1:A:88:LEU:HA	1:A:187:VAL:HG12	1.84	0.60
1:B:74:THR:HG22	1:B:91:VAL:HB	1.83	0.60
1:B:245:PHE:C	1:B:245:PHE:CD1	2.78	0.60
1:A:130:SER:O	1:A:133:GLN:HG2	2.00	0.60
1:A:57:ASP:OD1	1:A:58:ALA:N	2.35	0.60
1:B:53:THR:O	1:B:53:THR:HG22	2.01	0.60
1:A:287:LEU:O	1:A:288:LEU:HB2	2.02	0.59
1:A:214:ILE:N	1:A:214:ILE:HD12	2.17	0.59
1:B:78:ALA:O	1:B:80:GLY:N	2.31	0.59
1:A:246:THR:O	1:A:247:VAL:HG13	2.02	0.59
1:A:258:GLN:NE2	1:A:258:GLN:N	2.45	0.59
1:B:136:ALA:CB	1:B:146:LEU:HD21	2.30	0.59
1:A:59:LEU:HB2	1:A:222:ALA:O	2.03	0.59
1:B:266:PRO:HB3	1:B:275:TYR:CE1	2.38	0.58
1:A:164:ASP:HA	1:A:167:ILE:HD12	1.85	0.58
1:B:45:ASP:CB	1:B:304:LYS:HG3	2.33	0.58
1:A:242:LYS:O	1:A:243:ALA:HB3	2.02	0.58
1:A:229:VAL:HG22	1:A:229:VAL:O	2.01	0.58
1:B:95:GLU:HA	1:B:98:GLU:OE1	2.04	0.58
1:B:122:LEU:O	1:B:126:ARG:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:H	1:B:241:GLN:NE2	2.01	0.58
1:B:237:LEU:CD1	1:B:298:ILE:HG21	2.32	0.58
1:B:72:LEU:HD12	1:B:199:THR:HG22	1.86	0.58
1:A:305:ASN:ND2	1:A:305:ASN:C	2.60	0.57
1:A:85:LYS:O	1:A:86:ASP:HB2	2.04	0.57
1:B:296:VAL:HG12	1:B:298:ILE:HD12	1.87	0.57
1:B:167:ILE:HG22	1:B:171:GLN:HG3	1.87	0.57
1:B:96:GLN:NE2	1:B:96:GLN:HA	2.18	0.56
1:B:132:GLN:O	1:B:146:LEU:HD21	2.05	0.56
1:A:122:LEU:HG	1:A:156:LYS:HB3	1.86	0.56
1:A:286:GLY:O	1:A:287:LEU:O	2.22	0.56
1:B:190:MET:HE1	1:B:219:ASP:H	1.70	0.56
1:B:244:TRP:HZ3	1:B:299:GLN:HG2	1.70	0.56
1:A:237:LEU:HD21	1:A:277:ALA:HB2	1.87	0.56
1:A:138:THR:O	1:A:138:THR:HG22	2.05	0.56
1:B:190:MET:HE1	1:B:219:ASP:N	2.21	0.56
1:B:235:ILE:HD12	1:B:235:ILE:H	1.69	0.56
1:B:266:PRO:HB3	1:B:275:TYR:CD1	2.41	0.56
1:A:180:ASN:O	1:A:183:TYR:HB2	2.05	0.56
1:B:89:LEU:HD11	1:B:188:ALA:HB2	1.88	0.56
1:B:283:ASN:N	1:B:284:PRO:HD3	2.20	0.55
1:B:85:LYS:HG2	1:B:86:ASP:N	2.21	0.55
1:B:109:MET:CA	1:B:112:ARG:HB2	2.30	0.55
1:A:246:THR:C	1:A:247:VAL:HG22	2.31	0.55
1:B:122:LEU:HD23	1:B:123:LYS:HE2	1.88	0.55
1:B:215:LEU:O	1:B:215:LEU:CD2	2.53	0.55
1:A:251:GLN:O	1:A:252:LEU:HD13	2.07	0.55
1:B:289:ARG:HG3	1:B:292:MET:HE3	1.88	0.55
1:A:108:LEU:HD13	1:A:108:LEU:O	2.07	0.55
1:A:130:SER:O	1:A:133:GLN:N	2.39	0.55
1:B:128:THR:O	1:B:129:TYR:C	2.49	0.55
1:B:168:LYS:HD3	1:B:168:LYS:O	2.07	0.55
1:B:282:PRO:C	1:B:284:PRO:HD3	2.32	0.55
1:A:46:LEU:HB2	1:A:308:THR:CG2	2.37	0.55
1:A:83:VAL:HG21	1:A:217:LEU:HD21	1.89	0.55
1:B:283:ASN:CG	1:B:283:ASN:O	2.49	0.55
1:A:46:LEU:HB2	1:A:308:THR:HG22	1.89	0.54
1:A:163:ILE:HG22	1:A:167:ILE:HD11	1.89	0.54
1:A:227:ALA:O	1:A:276:TYR:HA	2.07	0.54
1:A:251:GLN:CD	1:A:251:GLN:H	2.14	0.54
1:A:260:LYS:HZ2	1:A:280:GLU:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:O	1:A:271:ASP:CB	2.55	0.54
1:B:142:SER:OG	1:B:143:GLN:N	2.34	0.54
1:B:224:LEU:HA	1:B:279:PHE:O	2.08	0.54
1:B:96:GLN:C	1:B:100:GLN:HE22	2.16	0.54
1:B:231:GLU:CD	1:B:273:ILE:HB	2.33	0.54
1:A:43:PRO:CB	1:A:305:ASN:HD21	2.21	0.53
1:A:51:LEU:HD21	1:A:297:HIS:ND1	2.23	0.53
1:A:79:ILE:HA	1:A:194:VAL:HG12	1.89	0.53
1:A:238:LYS:H	1:A:241:GLN:CD	2.16	0.53
1:B:175:ASP:O	1:B:179:THR:HB	2.07	0.53
1:B:230:SER:HB3	1:B:233:ASP:OD2	2.09	0.53
1:B:46:LEU:HD22	1:B:47:GLN:N	2.23	0.53
1:B:186:ILE:N	1:B:186:ILE:HD12	2.23	0.53
1:A:229:VAL:HG11	1:A:237:LEU:CD2	2.38	0.53
1:B:46:LEU:HD13	1:B:46:LEU:C	2.33	0.53
1:B:235:ILE:HD12	1:B:235:ILE:N	2.24	0.53
1:A:243:ALA:CA	1:A:297:HIS:O	2.52	0.53
1:B:198:THR:HB	1:B:213:ASN:ND2	2.20	0.53
1:A:134:ARG:C	1:A:136:ALA:N	2.64	0.52
1:A:279:PHE:CD1	1:A:279:PHE:N	2.78	0.52
1:B:205:VAL:HG23	1:B:212:PRO:HB3	1.92	0.52
1:A:52:ALA:HB1	1:A:228:GLN:O	2.10	0.52
1:A:94:PRO:HA	1:A:184:THR:HG21	1.91	0.52
1:B:69:SER:O	1:B:92:ILE:HG21	2.10	0.52
1:B:50:VAL:HG12	1:B:50:VAL:O	2.10	0.52
1:A:62:VAL:HG12	1:A:63:ASP:N	2.25	0.52
1:A:92:ILE:HD11	1:A:186:ILE:HD11	1.91	0.52
1:A:186:ILE:HD13	1:A:214:ILE:HG12	1.90	0.52
1:B:225:VAL:HG11	1:B:245:PHE:CE2	2.44	0.52
1:B:72:LEU:HD13	1:B:200:LEU:O	2.10	0.52
1:B:163:ILE:O	1:B:166:GLN:N	2.43	0.52
1:A:207:ALA:O	1:A:208:ALA:C	2.54	0.51
1:A:95:GLU:HA	1:A:98:GLU:HG3	1.92	0.51
1:A:79:ILE:HG23	1:A:194:VAL:O	2.11	0.51
1:A:258:GLN:H	1:A:258:GLN:HE21	1.55	0.51
1:B:235:ILE:H	1:B:235:ILE:CD1	2.23	0.51
1:A:105:GLU:CG	1:A:174:LEU:HD11	2.40	0.50
1:A:215:LEU:C	1:A:215:LEU:HD23	2.36	0.50
1:A:62:VAL:HG11	1:A:189:PRO:CG	2.41	0.50
1:A:143:GLN:O	1:A:144:GLN:C	2.54	0.50
1:B:56:LEU:HD12	1:B:224:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:HE21	1:B:63:ASP:H	1.60	0.50
1:A:214:ILE:HD12	1:A:214:ILE:H	1.77	0.50
1:B:130:SER:O	1:B:132:GLN:N	2.45	0.50
1:B:306:VAL:HG22	1:B:307:LEU:N	2.27	0.50
1:A:241:GLN:O	1:A:242:LYS:O	2.31	0.49
1:A:126:ARG:CB	1:A:153:MET:HE3	2.40	0.49
1:B:88:LEU:C	1:B:88:LEU:HD23	2.37	0.49
1:B:252:LEU:HD12	1:B:254:ARG:HG3	1.93	0.49
1:A:55:LYS:HD2	1:A:291:ASP:OD1	2.12	0.49
1:A:57:ASP:O	1:A:224:LEU:N	2.45	0.49
1:A:56:LEU:HD12	1:A:292:MET:O	2.11	0.49
1:A:108:LEU:O	1:A:108:LEU:CD1	2.60	0.49
1:B:290:LEU:N	1:B:290:LEU:HD12	2.26	0.49
1:A:45:ASP:OD2	1:A:305:ASN:N	2.43	0.49
1:A:51:LEU:CD2	1:A:297:HIS:ND1	2.76	0.49
1:A:94:PRO:HB2	1:A:181:LEU:HD11	1.93	0.49
1:A:175:ASP:O	1:A:179:THR:HG23	2.13	0.49
1:A:178:LYS:C	1:A:180:ASN:H	2.21	0.49
1:A:209:GLN:O	1:A:210:GLN:HB2	2.12	0.49
1:A:213:ASN:C	1:A:213:ASN:HD22	2.21	0.49
1:B:224:LEU:HD22	1:B:279:PHE:O	2.13	0.49
1:B:74:THR:HA	1:B:201:GLN:HE21	1.74	0.49
1:B:135:LEU:CD2	1:B:140:ALA:HB2	2.25	0.49
1:B:196:GLN:HB3	1:B:216:THR:CG2	2.43	0.49
1:B:226:LYS:HD3	1:B:278:ARG:HG2	1.95	0.49
1:A:88:LEU:CD1	1:A:185:ARG:HB3	2.43	0.48
1:B:250:ASP:O	1:B:250:ASP:OD1	2.30	0.48
1:B:94:PRO:O	1:B:96:GLN:N	2.45	0.48
1:A:47:GLN:HA	1:A:301:THR:HG23	1.94	0.48
1:B:293:THR:HG22	1:B:294:ALA:N	2.28	0.48
1:A:78:ALA:HA	1:A:197:ILE:HD11	1.95	0.48
1:A:233:ASP:OD2	1:A:233:ASP:N	2.46	0.48
1:A:306:VAL:O	1:A:306:VAL:HG12	2.14	0.48
1:B:293:THR:CG2	1:B:294:ALA:N	2.77	0.48
1:A:121:GLU:HB3	1:A:156:LYS:HE2	1.96	0.48
1:A:206:ILE:HG22	1:B:211:ALA:HB2	1.95	0.48
1:A:279:PHE:N	1:A:279:PHE:HD1	2.12	0.48
1:A:101:ILE:O	1:A:102:LYS:C	2.56	0.48
1:B:115:ARG:HA	1:B:163:ILE:CD1	2.43	0.48
1:B:141:VAL:HG23	1:B:145:ASP:HB2	1.96	0.48
1:B:198:THR:CB	1:B:213:ASN:ND2	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:SER:CB	1:A:206:ILE:HA	2.43	0.47
1:A:237:LEU:HD13	1:A:298:ILE:HD12	1.95	0.47
1:A:269:VAL:C	1:A:270:ASN:CG	2.82	0.47
1:A:142:SER:OG	1:A:143:GLN:N	2.46	0.47
1:B:89:LEU:HD11	1:B:188:ALA:CA	2.45	0.47
1:B:289:ARG:HG3	1:B:292:MET:CE	2.44	0.47
1:A:244:TRP:CE3	1:A:254:ARG:HD3	2.50	0.47
1:A:47:GLN:HB2	1:A:301:THR:C	2.39	0.47
1:A:130:SER:O	1:A:131:ARG:C	2.57	0.47
1:B:180:ASN:HA	1:B:183:TYR:CD2	2.46	0.47
1:B:108:LEU:HD11	1:B:170:ASN:HB3	1.97	0.47
1:B:205:VAL:HG21	1:B:212:PRO:CB	2.45	0.47
1:B:209:GLN:HB3	1:B:210:GLN:OE1	2.15	0.47
1:A:72:LEU:HD22	1:A:201:GLN:HA	1.97	0.47
1:A:269:VAL:O	1:A:270:ASN:CG	2.58	0.47
1:A:203:GLN:HG2	1:B:63:ASP:O	2.14	0.47
1:A:106:ALA:HB2	1:B:168:LYS:HD2	1.96	0.46
1:B:186:ILE:N	1:B:186:ILE:CD1	2.79	0.46
1:B:60:ARG:HH12	1:B:219:ASP:CG	2.23	0.46
1:B:205:VAL:CG2	1:B:212:PRO:HB3	2.45	0.46
1:B:238:LYS:O	1:B:239:PRO:C	2.58	0.46
1:A:72:LEU:CD1	1:A:199:THR:HG22	2.45	0.46
1:A:258:GLN:N	1:A:258:GLN:CD	2.72	0.46
1:A:133:GLN:O	1:A:136:ALA:HB3	2.14	0.46
1:A:162:THR:HG22	1:A:166:GLN:HE22	1.79	0.46
1:A:251:GLN:OE1	1:A:251:GLN:N	2.43	0.46
1:A:242:LYS:CD	1:A:242:LYS:N	2.65	0.46
1:A:304:LYS:O	1:A:305:ASN:HB3	2.14	0.46
1:A:124:LEU:HD22	1:B:151:THR:OG1	2.15	0.46
1:B:52:ALA:N	1:B:296:VAL:O	2.47	0.46
1:B:240:GLY:HA2	1:B:258:GLN:HB3	1.97	0.46
1:A:47:GLN:N	1:A:47:GLN:OE1	2.48	0.46
1:B:129:TYR:O	1:B:130:SER:C	2.59	0.46
1:B:135:LEU:HD22	1:B:140:ALA:CB	2.25	0.46
1:A:121:GLU:HB3	1:A:156:LYS:CE	2.46	0.46
1:A:163:ILE:O	1:A:167:ILE:HG13	2.16	0.46
1:A:269:VAL:O	1:A:270:ASN:ND2	2.49	0.46
1:B:299:GLN:O	1:B:300:LEU:C	2.59	0.46
1:B:149:ALA:O	1:B:152:GLU:HB3	2.15	0.46
1:B:229:VAL:HG22	1:B:230:SER:N	2.30	0.46
1:B:174:LEU:O	1:B:178:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD13	1:A:199:THR:HG22	1.98	0.45
1:A:76:SER:O	1:A:77:VAL:HG13	2.16	0.45
1:B:108:LEU:CD1	1:B:170:ASN:HB3	2.46	0.45
1:B:128:THR:HG23	1:B:132:GLN:HG2	1.98	0.45
1:B:237:LEU:CA	1:B:241:GLN:HE22	2.14	0.45
1:A:43:PRO:CB	1:A:305:ASN:ND2	2.77	0.45
1:A:119:GLU:O	1:A:123:LYS:HG3	2.16	0.45
1:B:242:LYS:HG3	1:B:258:GLN:OE1	2.16	0.45
1:A:163:ILE:O	1:A:166:GLN:HB2	2.17	0.45
1:A:286:GLY:O	1:A:287:LEU:C	2.59	0.45
1:A:225:VAL:HB	1:A:279:PHE:CE1	2.52	0.45
1:B:242:LYS:HA	1:B:257:GLY:O	2.15	0.45
1:B:290:LEU:N	1:B:290:LEU:CD1	2.80	0.45
1:A:229:VAL:HG11	1:A:237:LEU:HD22	1.99	0.45
1:A:47:GLN:HA	1:A:301:THR:CG2	2.47	0.45
1:A:127:VAL:O	1:A:128:THR:C	2.60	0.45
1:B:51:LEU:HA	1:B:297:HIS:HA	1.99	0.45
1:B:115:ARG:HB2	1:B:163:ILE:HG21	1.97	0.45
1:B:253:THR:HG22	1:B:253:THR:O	2.17	0.45
1:B:136:ALA:HA	1:B:140:ALA:H	1.82	0.45
1:B:244:TRP:CZ3	1:B:299:GLN:HG2	2.52	0.45
1:A:249:GLY:O	1:A:250:ASP:CB	2.65	0.45
1:A:261:ASP:O	1:A:262:VAL:HG23	2.17	0.45
1:A:69:SER:OG	1:A:206:ILE:HD12	2.18	0.44
1:B:85:LYS:HG2	1:B:86:ASP:H	1.82	0.44
1:A:287:LEU:O	1:A:288:LEU:CB	2.66	0.44
1:A:60:ARG:O	1:A:218:ALA:HA	2.16	0.44
1:B:107:THR:HG21	1:B:170:ASN:HD22	1.79	0.44
1:A:128:THR:O	1:A:132:GLN:HG3	2.18	0.44
1:B:305:ASN:O	1:B:306:VAL:HB	2.17	0.44
1:A:46:LEU:HD23	1:A:308:THR:HG21	1.99	0.44
1:A:302:ASP:O	1:A:303:VAL:C	2.60	0.44
1:A:138:THR:O	1:A:139:GLN:O	2.36	0.44
1:A:139:GLN:C	1:A:139:GLN:CD	2.85	0.44
1:A:220:MET:O	1:A:221:SER:C	2.60	0.44
1:B:111:LEU:HD13	1:B:166:GLN:HB3	1.99	0.44
1:A:70:GLY:HA2	1:B:67:GLN:OE1	2.16	0.43
1:A:141:VAL:CG2	1:A:145:ASP:HB2	2.48	0.43
1:A:157:GLN:C	1:A:159:GLN:H	2.26	0.43
1:B:126:ARG:HG3	1:B:153:MET:SD	2.58	0.43
1:B:96:GLN:C	1:B:100:GLN:NE2	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ASN:C	1:A:306:VAL:HG23	2.43	0.43
1:B:269:VAL:O	1:B:269:VAL:CG2	2.59	0.43
1:A:241:GLN:NE2	1:A:300:LEU:HA	2.33	0.43
1:A:242:LYS:O	1:A:243:ALA:CB	2.66	0.43
1:B:74:THR:HG23	1:B:91:VAL:HB	1.96	0.43
1:A:100:GLN:O	1:A:104:VAL:HG23	2.19	0.43
1:A:229:VAL:O	1:A:229:VAL:CG2	2.66	0.43
1:A:236:HIS:CB	1:A:300:LEU:HD13	2.47	0.43
1:B:169:ARG:O	1:B:172:ALA:HB3	2.18	0.43
1:B:105:GLU:O	1:B:108:LEU:HB2	2.19	0.43
1:B:56:LEU:HD11	1:B:223:MET:HB3	1.99	0.43
1:B:225:VAL:HG13	1:B:279:PHE:HB3	2.00	0.43
1:B:266:PRO:HB2	1:B:274:PHE:O	2.18	0.43
1:B:302:ASP:OD1	1:B:302:ASP:O	2.37	0.43
1:A:56:LEU:HA	1:A:224:LEU:O	2.19	0.43
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.74	0.43
1:B:199:THR:HB	1:B:214:ILE:HA	1.99	0.43
1:B:85:LYS:O	1:B:86:ASP:HB2	2.18	0.43
1:A:110:GLU:O	1:A:114:GLN:CG	2.67	0.42
1:A:43:PRO:N	1:A:307:LEU:HG	2.35	0.42
1:A:193:GLU:O	1:A:217:LEU:HA	2.19	0.42
1:B:108:LEU:O	1:B:112:ARG:N	2.52	0.42
1:B:114:GLN:HE21	1:B:114:GLN:HB2	1.66	0.42
1:A:164:ASP:OD2	1:A:167:ILE:HD12	2.19	0.42
1:B:133:GLN:O	1:B:136:ALA:HB3	2.19	0.42
1:A:94:PRO:O	1:A:97:ALA:N	2.51	0.42
1:A:266:PRO:HB2	1:A:273:ILE:HG13	2.00	0.42
1:B:296:VAL:HG12	1:B:298:ILE:CD1	2.48	0.42
1:A:63:ASP:CG	1:A:216:THR:HB	2.45	0.42
1:A:141:VAL:O	1:A:142:SER:OG	2.25	0.42
1:A:79:ILE:H	1:A:79:ILE:HG13	1.65	0.42
1:A:96:GLN:HE21	1:B:176:THR:HG23	1.85	0.42
1:B:101:ILE:O	1:B:105:GLU:HG3	2.20	0.42
1:B:188:ALA:HB1	1:B:217:LEU:HD11	2.01	0.42
1:B:226:LYS:NZ	1:B:278:ARG:CD	2.65	0.42
1:B:288:LEU:HA	1:B:292:MET:SD	2.60	0.42
1:A:203:GLN:CG	1:B:63:ASP:O	2.68	0.42
1:B:94:PRO:O	1:B:95:GLU:C	2.63	0.42
1:A:92:ILE:O	1:A:94:PRO:HD3	2.20	0.41
1:A:213:ASN:C	1:A:213:ASN:ND2	2.76	0.41
1:B:92:ILE:O	1:B:94:PRO:CD	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ARG:HB2	1:B:275:TYR:OH	2.21	0.41
1:A:50:VAL:HB	1:A:298:ILE:CD1	2.37	0.41
1:A:127:VAL:C	1:A:129:TYR:N	2.73	0.41
1:A:242:LYS:HD3	1:A:299:GLN:CB	2.39	0.41
1:A:249:GLY:O	1:B:235:ILE:HG12	2.20	0.41
1:A:269:VAL:HB	1:A:274:PHE:CE2	2.56	0.41
1:B:167:ILE:O	1:B:168:LYS:C	2.63	0.41
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.84	0.41
1:A:79:ILE:HA	1:A:194:VAL:CG1	2.51	0.41
1:B:143:GLN:O	1:B:144:GLN:C	2.64	0.41
1:A:49:SER:HA	1:A:298:ILE:O	2.21	0.41
1:A:62:VAL:CG1	1:A:63:ASP:N	2.84	0.41
1:A:96:GLN:NE2	1:B:176:THR:HG23	2.36	0.41
1:A:114:GLN:O	1:A:115:ARG:C	2.61	0.41
1:A:139:GLN:O	1:A:140:ALA:HB2	2.21	0.41
1:B:42:ARG:HA	1:B:43:PRO:HD3	1.91	0.41
1:B:72:LEU:HD12	1:B:199:THR:CG2	2.51	0.41
1:A:226:LYS:HG2	1:A:278:ARG:HD3	2.02	0.40
1:A:229:VAL:HG11	1:A:237:LEU:HD21	2.01	0.40
1:B:271:ASP:O	1:B:272:ALA:O	2.40	0.40
1:A:93:ASP:OD1	1:A:93:ASP:C	2.63	0.40
1:B:59:LEU:HD23	1:B:219:ASP:OD2	2.21	0.40
1:B:236:HIS:O	1:B:237:LEU:CB	2.69	0.40
1:B:238:LYS:HD2	1:B:238:LYS:HA	1.96	0.40
1:B:113:ALA:O	1:B:116:GLN:N	2.55	0.40
1:B:298:ILE:HG22	1:B:299:GLN:N	2.36	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	264/341 (77%)	207 (78%)	39 (15%)	18 (7%)	1	5
1	B	265/341 (78%)	203 (77%)	39 (15%)	23 (9%)	0	3
All	All	529/682 (78%)	410 (78%)	78 (15%)	41 (8%)	1	4

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ALA
1	A	221	SER
1	A	242	LYS
1	A	247	VAL
1	A	252	LEU
1	A	254	ARG
1	A	271	ASP
1	A	287	LEU
1	B	79	ILE
1	B	139	GLN
1	B	254	ARG
1	B	287	LEU
1	A	95	GLU
1	A	144	GLN
1	A	208	ALA
1	A	250	ASP
1	A	306	VAL
1	B	50	VAL
1	B	95	GLU
1	B	130	SER
1	B	131	ARG
1	B	242	LYS
1	B	272	ALA
1	A	139	GLN
1	A	210	GLN
1	B	80	GLY
1	B	194	VAL
1	B	251	GLN
1	B	305	ASN
1	B	306	VAL
1	A	86	ASP
1	A	142	SER
1	A	243	ALA
1	B	239	PRO
1	B	261	ASP

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Mol	Chain	Res	Type
1	B	288	LEU
1	B	212	PRO
1	B	237	LEU
1	B	240	GLY
1	B	284	PRO
1	B	141	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/281 (79%)	190 (86%)	31 (14%)	3	16
1	B	222/281 (79%)	192 (86%)	30 (14%)	4	18
All	All	443/562 (79%)	382 (86%)	61 (14%)	3	17

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	81	ASP
1	A	91	VAL
1	A	108	LEU
1	A	111	LEU
1	A	122	LEU
1	A	152	GLU
1	A	153	MET
1	A	159	GLN
1	A	160	ILE
1	A	173	SER
1	A	180	ASN
1	A	198	THR
1	A	206	ILE
1	A	213	ASN
1	A	215	LEU
1	A	216	THR

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Mol	Chain	Res	Type
1	A	229	VAL
1	A	244	TRP
1	A	247	VAL
1	A	251	GLN
1	A	252	LEU
1	A	256	GLU
1	A	258	GLN
1	A	265	THR
1	A	270	ASN
1	A	279	PHE
1	A	287	LEU
1	A	293	THR
1	A	301	THR
1	A	307	LEU
1	B	50	VAL
1	B	51	LEU
1	B	57	ASP
1	B	64	VAL
1	B	92	ILE
1	B	108	LEU
1	B	112	ARG
1	B	115	ARG
1	B	127	VAL
1	B	128	THR
1	B	130	SER
1	B	148	ASN
1	B	152	GLU
1	B	166	GLN
1	B	174	LEU
1	B	179	THR
1	B	195	THR
1	B	200	LEU
1	B	210	GLN
1	B	215	LEU
1	B	216	THR
1	B	220	MET
1	B	225	VAL
1	B	241	GLN
1	B	251	GLN
1	B	265	THR
1	B	279	PHE
1	B	280	GLU

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Mol	Chain	Res	Type
1	B	299	GLN
1	B	303	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	133	GLN
1	A	148	ASN
1	A	159	GLN
1	A	166	GLN
1	A	180	ASN
1	A	203	GLN
1	A	213	ASN
1	A	258	GLN
1	A	283	ASN
1	A	299	GLN
1	A	305	ASN
1	B	96	GLN
1	B	100	GLN
1	B	114	GLN
1	B	116	GLN
1	B	133	GLN
1	B	143	GLN
1	B	144	GLN
1	B	148	ASN
1	B	170	ASN
1	B	201	GLN
1	B	209	GLN
1	B	213	ASN
1	B	241	GLN
1	B	251	GLN
1	B	299	GLN
1	B	305	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	266/341 (78%)	-1.63	0 100 100	10, 28, 60, 75	0
1	B	267/341 (78%)	-1.61	0 100 100	9, 28, 51, 69	0
All	All	533/682 (78%)	-1.62	0 100 100	9, 28, 57, 75	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.