



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:16 AM UTC

PDB ID : 2JLF / pdb_00002jlf
Title : STRUCTURAL EXPLANATION FOR THE ROLE OF MN IN THE ACTIVITY OF PHI6 RNA- DEPENDENT RNA POLYMERASE
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Deposited on : 2008-09-08
Resolution : 3.20 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

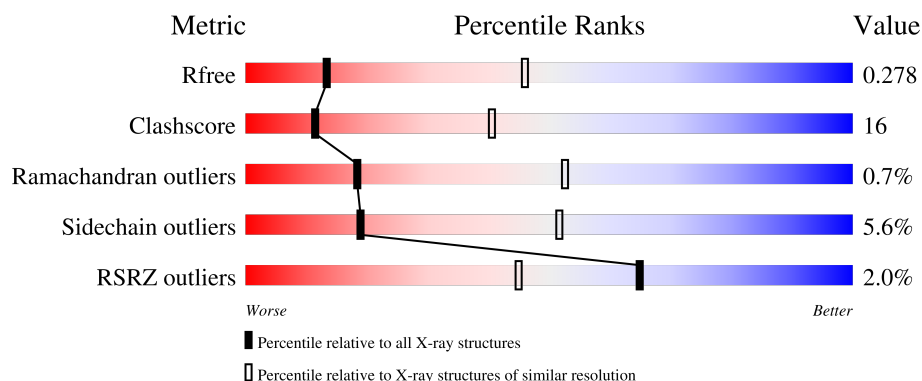
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	664	4% 63% 32% ..
1	B	664	64% 32% .
1	C	664	4% 63% 31% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15610 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 RNA-DIRECTED RNA POLYMERASE.

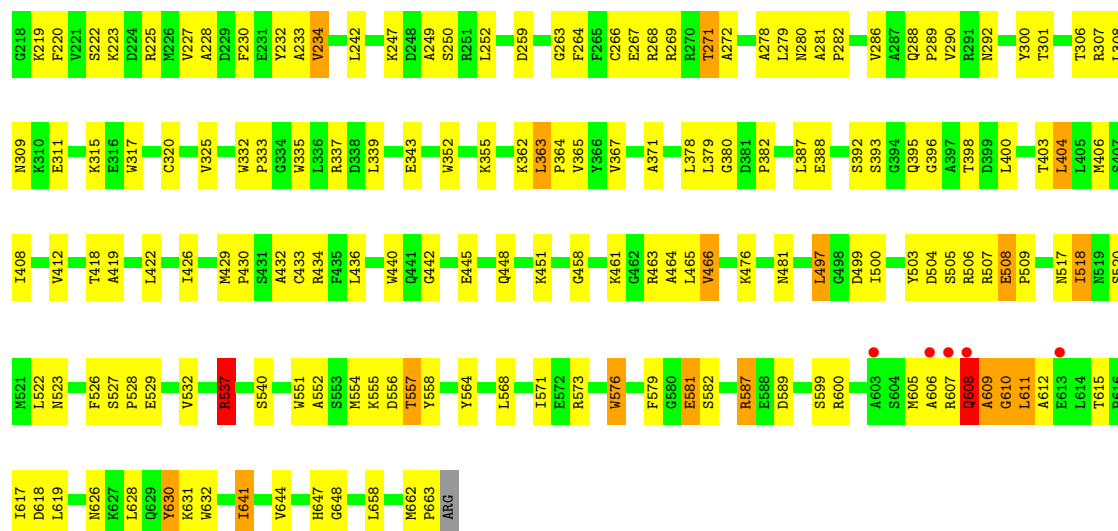
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5186	3297	895	963	31			
1	B	661	Total	C	N	O	S	0	0	0
			5235	3325	906	972	32			
1	C	654	Total	C	N	O	S	0	0	0
			5187	3298	895	963	31			

There are 6 discrepancies between the modelled and reference sequences:

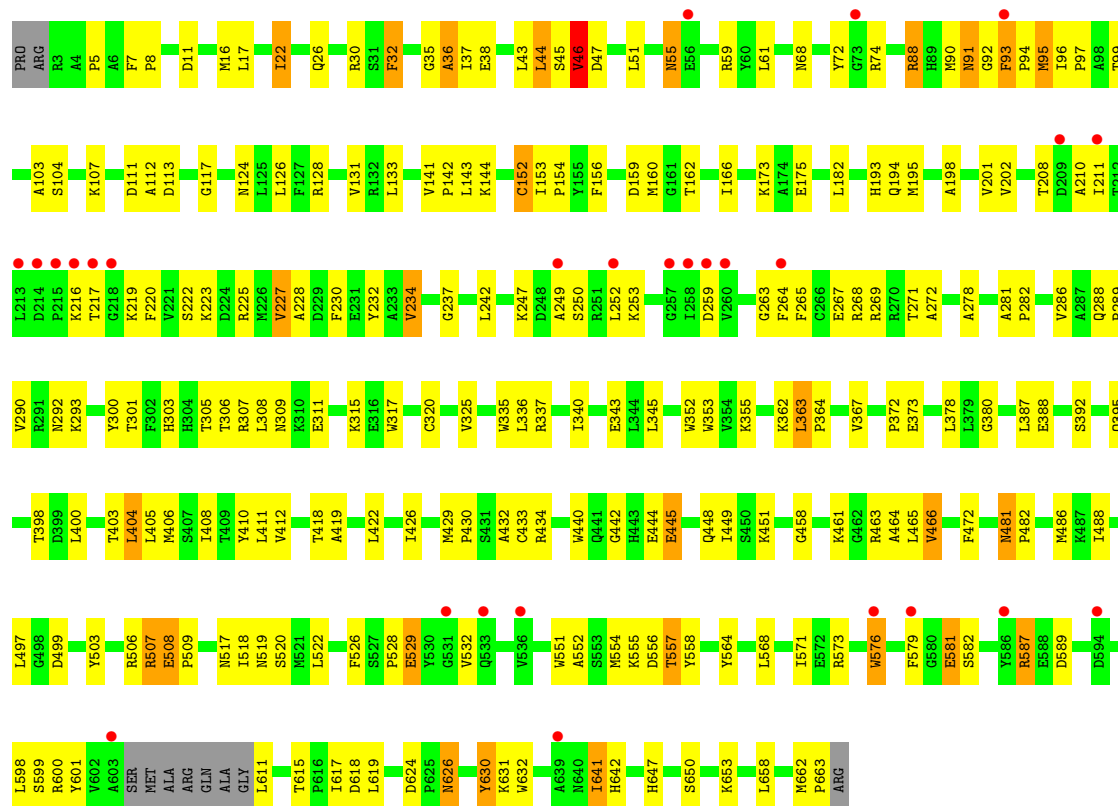
Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
A	491	GLN	GLU	engineered mutation	UNP P11124
B	456	MET	ILE	conflict	UNP P11124
B	491	GLN	GLU	engineered mutation	UNP P11124
C	456	MET	ILE	conflict	UNP P11124
C	491	GLN	GLU	engineered mutation	UNP P11124

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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



● Molecule 1: RNA-DIRECTED RNA POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	110.04Å 110.04Å 159.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.02 – 3.20 18.02 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (18.02-3.20) 99.4 (18.02-3.20)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.21Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.228 , 0.286 0.216 , 0.278	Depositor DCC
R_{free} test set	1772 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.049 for h,-h-k,-l 0.031 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15610	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/5315	0.93	18/7190 (0.3%)
1	B	0.49	0/5365	0.91	15/7258 (0.2%)
1	C	0.43	0/5316	0.92	14/7192 (0.2%)
All	All	0.47	0/15996	0.92	47/21640 (0.2%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	PHE	CA-C-N	13.38	134.28	119.83
1	C	93	PHE	C-N-CA	13.38	134.28	119.83
1	A	506	ARG	NE-CZ-NH2	12.05	130.05	119.20
1	A	269	ARG	NE-CZ-NH2	10.91	129.02	119.20
1	B	204	ARG	NE-CZ-NH2	10.55	128.69	119.20
1	A	506	ARG	NE-CZ-NH1	-10.45	111.05	121.50
1	B	537	ARG	CB-CG-CD	10.28	134.94	111.30
1	A	307	ARG	NE-CZ-NH2	10.00	128.20	119.20
1	C	88	ARG	NE-CZ-NH2	10.00	128.20	119.20
1	B	204	ARG	NE-CZ-NH1	-9.89	111.61	121.50
1	A	269	ARG	NE-CZ-NH1	-9.82	111.67	121.50
1	A	307	ARG	NE-CZ-NH1	-9.75	111.75	121.50
1	C	88	ARG	NE-CZ-NH1	-9.33	112.17	121.50
1	A	506	ARG	CD-NE-CZ	8.68	136.55	124.40
1	B	30	ARG	NE-CZ-NH2	8.28	126.65	119.20
1	B	30	ARG	NE-CZ-NH1	-7.79	113.71	121.50
1	C	88	ARG	CD-NE-CZ	7.61	135.06	124.40
1	B	204	ARG	CD-NE-CZ	7.30	134.63	124.40
1	A	307	ARG	CD-NE-CZ	7.25	134.55	124.40
1	A	269	ARG	CD-NE-CZ	7.23	134.52	124.40
1	A	481	ASN	CA-C-N	6.54	126.12	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ASN	C-N-CA	6.54	126.12	119.19
1	C	481	ASN	CA-C-N	6.46	126.04	119.19
1	C	481	ASN	C-N-CA	6.46	126.04	119.19
1	A	47	ASP	CA-C-N	6.39	127.82	119.84
1	A	47	ASP	C-N-CA	6.39	127.82	119.84
1	B	47	ASP	CA-C-N	6.19	127.58	119.84
1	B	47	ASP	C-N-CA	6.19	127.58	119.84
1	B	481	ASN	CA-C-N	6.18	125.74	119.19
1	B	481	ASN	C-N-CA	6.18	125.74	119.19
1	C	508	GLU	CA-C-N	6.08	125.77	119.56
1	C	508	GLU	C-N-CA	6.08	125.77	119.56
1	C	47	ASP	CA-C-N	5.92	127.24	119.84
1	C	47	ASP	C-N-CA	5.92	127.24	119.84
1	C	46	VAL	N-CA-CB	-5.88	104.46	112.28
1	A	508	GLU	CA-C-N	5.48	125.15	119.56
1	A	508	GLU	C-N-CA	5.48	125.15	119.56
1	A	30	ARG	N-CA-C	5.37	118.10	110.10
1	C	152	CYS	CB-CA-C	-5.37	109.41	115.79
1	B	201	VAL	CB-CA-C	-5.36	106.58	112.68
1	B	537	ARG	CA-CB-CG	-5.33	103.44	114.10
1	A	46	VAL	CB-CA-C	-5.30	106.09	112.19
1	B	508	GLU	CA-C-N	5.27	124.93	119.56
1	B	508	GLU	C-N-CA	5.27	124.93	119.56
1	B	608	GLN	N-CA-C	5.16	113.70	108.75
1	A	450	SER	N-CA-C	5.09	116.15	108.46
1	C	198	ALA	N-CA-C	5.06	116.21	108.42

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	5186	0	5080	168	2
1	B	5235	0	5131	162	0
1	C	5187	0	5082	170	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	15610	0	15293	496	2

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 16.

All (496) 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:95:MET:HE2	1:A:269:ARG:H	1.26	0.97
1:B:95:MET:HE2	1:B:269:ARG:H	1.28	0.96
1:B:364:PRO:HA	1:B:387:LEU:CD1	1.96	0.96
1:B:99:THR:HB	1:B:227:VAL:HG12	1.50	0.93
1:C:364:PRO:HA	1:C:387:LEU:CD1	1.99	0.91
1:C:95:MET:HE2	1:C:269:ARG:H	1.35	0.90
1:B:364:PRO:HA	1:B:387:LEU:HD12	1.53	0.89
1:A:364:PRO:HA	1:A:387:LEU:CD1	2.01	0.89
1:A:160:MET:HE3	1:A:647:HIS:HB3	1.55	0.86
1:C:364:PRO:HA	1:C:387:LEU:HD12	1.57	0.85
1:A:364:PRO:HA	1:A:387:LEU:HD12	1.56	0.85
1:B:126:LEU:HD21	1:B:426:ILE:HD13	1.58	0.84
1:C:461:LYS:HA	1:C:465:LEU:HD22	1.58	0.84
1:C:99:THR:HB	1:C:227:VAL:HG12	1.61	0.82
1:B:160:MET:HE3	1:B:647:HIS:HB3	1.61	0.82
1:A:126:LEU:HD21	1:A:426:ILE:HD13	1.62	0.80
1:C:126:LEU:HD21	1:C:426:ILE:HD13	1.65	0.78
1:B:461:LYS:HA	1:B:465:LEU:HD22	1.64	0.77
1:C:220:PHE:CD2	1:C:263:GLY:HA3	2.19	0.77
1:A:72:TYR:CZ	1:A:476:LYS:HE2	2.20	0.76
1:A:461:LYS:HA	1:A:465:LEU:HD22	1.66	0.76
1:C:35:GLY:HA2	1:C:93:PHE:CZ	2.21	0.75
1:A:202:VAL:HG23	1:A:272:ALA:HB3	1.68	0.73
1:A:658:LEU:HG	1:A:662:MET:HE2	1.68	0.73
1:C:202:VAL:HG23	1:C:272:ALA:HB3	1.69	0.73
1:A:93:PHE:CG	1:A:252:LEU:HD21	2.24	0.72
1:A:249:ALA:O	1:A:252:LEU:HB2	1.90	0.72
1:C:658:LEU:HG	1:C:662:MET:HE2	1.70	0.72
1:A:90:MET:HE2	1:A:264:PHE:HB3	1.72	0.72
1:B:337:ARG:NH1	1:B:362:LYS:HG2	2.05	0.72
1:C:90:MET:HE2	1:C:264:PHE:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:NH2	1:C:253:LYS:HZ2	1.89	0.71
1:C:220:PHE:HD2	1:C:263:GLY:HA3	1.54	0.71
1:B:220:PHE:CD2	1:B:263:GLY:HA3	2.26	0.70
1:A:220:PHE:CD2	1:A:263:GLY:HA3	2.28	0.69
1:A:537:ARG:NH2	1:C:253:LYS:NZ	2.39	0.69
1:B:658:LEU:HG	1:B:662:MET:HE2	1.73	0.69
1:C:38:GLU:HB3	1:C:532:VAL:HG22	1.73	0.68
1:B:38:GLU:HB3	1:B:532:VAL:HG22	1.76	0.68
1:B:551:TRP:CH2	1:B:554:MET:HE1	2.29	0.68
1:C:249:ALA:O	1:C:252:LEU:HB2	1.92	0.68
1:C:337:ARG:NH1	1:C:362:LYS:HG2	2.08	0.68
1:C:124:ASN:O	1:C:128:ARG:HG3	1.94	0.67
1:B:552:ALA:HB3	1:B:619:LEU:HD13	1.74	0.67
1:C:551:TRP:CH2	1:C:554:MET:HE1	2.29	0.67
1:C:107:LYS:HE3	1:C:111:ASP:OD2	1.95	0.67
1:A:552:ALA:HB3	1:A:619:LEU:HD13	1.76	0.67
1:A:551:TRP:CH2	1:A:554:MET:HE1	2.30	0.66
1:C:131:VAL:HG11	1:C:343:GLU:HB3	1.77	0.66
1:C:195:MET:HE2	1:C:278:ALA:O	1.95	0.65
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.31	0.65
1:B:93:PHE:CG	1:B:252:LEU:HD21	2.32	0.65
1:B:540:SER:HB2	1:B:644:VAL:O	1.97	0.65
1:C:307:ARG:HG2	1:C:499:ASP:OD2	1.96	0.65
1:A:17:LEU:HD11	1:A:378:LEU:HD22	1.78	0.65
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.32	0.64
1:A:223:LYS:HD3	1:A:225:ARG:HH21	1.63	0.64
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.32	0.64
1:B:124:ASN:O	1:B:128:ARG:HG3	1.97	0.64
1:C:95:MET:C	1:C:96:ILE:HG13	2.23	0.64
1:A:576:TRP:CD1	1:A:581:GLU:O	2.51	0.63
1:C:576:TRP:CD1	1:C:581:GLU:O	2.52	0.63
1:A:17:LEU:HB3	1:A:153:ILE:HD13	1.80	0.63
1:B:162:THR:O	1:B:166:ILE:HG13	1.98	0.63
1:A:38:GLU:HB3	1:A:532:VAL:HG22	1.80	0.63
1:A:90:MET:HE2	1:A:264:PHE:CB	2.29	0.63
1:B:107:LYS:HE3	1:B:111:ASP:OD2	1.99	0.63
1:C:223:LYS:HD3	1:C:225:ARG:HH21	1.63	0.63
1:B:131:VAL:HG11	1:B:343:GLU:HB3	1.80	0.63
1:C:395:GLN:O	1:C:398:THR:HG22	1.99	0.62
1:A:220:PHE:HD2	1:A:263:GLY:HA3	1.65	0.62
1:C:17:LEU:HD11	1:C:378:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PHE:HD2	1:B:263:GLY:HA3	1.64	0.62
1:C:141:VAL:HG11	1:C:292:ASN:ND2	2.15	0.62
1:B:17:LEU:HD11	1:B:378:LEU:HD22	1.82	0.62
1:A:107:LYS:HE3	1:A:111:ASP:OD2	2.00	0.61
1:C:94:PRO:HB3	1:C:269:ARG:HH11	1.65	0.61
1:A:93:PHE:CD2	1:A:252:LEU:HD21	2.35	0.61
1:C:162:THR:O	1:C:166:ILE:HG13	2.00	0.61
1:A:124:ASN:O	1:A:128:ARG:HG3	2.00	0.61
1:A:8:PRO:HD2	1:A:11:ASP:HB2	1.81	0.61
1:A:17:LEU:O	1:A:153:ILE:HG23	1.99	0.61
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.36	0.61
1:B:230:PHE:O	1:B:234:VAL:HG22	2.00	0.61
1:C:17:LEU:HB3	1:C:153:ILE:HD13	1.83	0.61
1:A:208:THR:HG21	1:A:523:ASN:CG	2.26	0.60
1:B:202:VAL:HG12	1:B:272:ALA:HB3	1.81	0.60
1:C:230:PHE:O	1:C:234:VAL:HG22	2.01	0.60
1:B:576:TRP:CD1	1:B:581:GLU:O	2.55	0.60
1:A:88:ARG:HD3	1:A:263:GLY:O	2.02	0.60
1:A:138:LEU:HB2	1:A:662:MET:SD	2.42	0.60
1:A:131:VAL:HG11	1:A:343:GLU:HB3	1.83	0.60
1:C:8:PRO:HD2	1:C:11:ASP:HB2	1.83	0.60
1:C:17:LEU:O	1:C:153:ILE:HG23	2.01	0.59
1:B:249:ALA:O	1:B:252:LEU:HB2	2.03	0.59
1:B:8:PRO:HD2	1:B:11:ASP:HB2	1.84	0.59
1:B:307:ARG:HG2	1:B:499:ASP:OD2	2.03	0.58
1:B:286:VAL:C	1:B:289:PRO:HD2	2.28	0.58
1:B:208:THR:HG21	1:B:523:ASN:CG	2.28	0.58
1:C:517:ASN:HB3	1:C:520:SER:OG	2.03	0.58
1:B:599:SER:HB2	1:B:606:ALA:C	2.29	0.58
1:C:43:LEU:HD12	1:C:44:LEU:N	2.18	0.58
1:C:600:ARG:O	1:C:600:ARG:HG2	2.03	0.58
1:A:99:THR:HB	1:A:227:VAL:HG12	1.85	0.58
1:A:88:ARG:HB2	1:A:211:ILE:HD12	1.87	0.57
1:C:94:PRO:HB3	1:C:269:ARG:HD3	1.87	0.57
1:B:194:GLN:O	1:B:278:ALA:HB3	2.04	0.57
1:C:141:VAL:HG11	1:C:292:ASN:HD21	1.69	0.57
1:B:95:MET:HE2	1:B:269:ARG:N	2.11	0.57
1:B:301:THR:HG23	1:B:440:TRP:O	2.05	0.57
1:C:306:THR:O	1:C:309:ASN:HB3	2.04	0.57
1:A:160:MET:HE3	1:A:647:HIS:CB	2.32	0.57
1:B:600:ARG:O	1:B:600:ARG:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ARG:HH11	1:C:507:ARG:HB3	1.70	0.57
1:B:364:PRO:CA	1:B:387:LEU:HD12	2.30	0.56
1:C:91:ASN:HA	1:C:267:GLU:OE1	2.05	0.56
1:A:337:ARG:NH1	1:A:362:LYS:HG2	2.20	0.56
1:B:609:ALA:O	1:B:610:GLY:C	2.48	0.56
1:A:90:MET:HE1	1:A:261:PRO:HD2	1.88	0.56
1:A:230:PHE:O	1:A:234:VAL:HG22	2.04	0.56
1:B:72:TYR:CE1	1:B:476:LYS:HE2	2.40	0.56
1:A:286:VAL:C	1:A:289:PRO:HD2	2.31	0.56
1:C:301:THR:HG22	1:C:448:GLN:O	2.05	0.56
1:C:552:ALA:HB3	1:C:619:LEU:HD13	1.86	0.56
1:A:600:ARG:HG2	1:A:600:ARG:O	2.05	0.56
1:A:117:GLY:HA2	1:A:335:TRP:CD2	2.40	0.55
1:B:195:MET:HE2	1:B:278:ALA:O	2.05	0.55
1:A:162:THR:O	1:A:166:ILE:HG13	2.06	0.55
1:B:90:MET:HE2	1:B:264:PHE:HB3	1.88	0.55
1:B:17:LEU:HB3	1:B:153:ILE:HD13	1.88	0.55
1:B:306:THR:O	1:B:309:ASN:HB3	2.07	0.55
1:B:395:GLN:O	1:B:398:THR:HG22	2.07	0.55
1:C:26:GLN:O	1:C:30:ARG:HG3	2.07	0.55
1:B:662:MET:HB3	1:B:663:PRO:CD	2.37	0.55
1:C:225:ARG:HD2	1:C:268:ARG:HD2	1.89	0.55
1:A:55:ASN:O	1:A:59:ARG:HG3	2.08	0.54
1:A:225:ARG:HD2	1:A:268:ARG:HD2	1.90	0.54
1:C:90:MET:HE2	1:C:264:PHE:CB	2.37	0.54
1:C:94:PRO:HB3	1:C:269:ARG:NH1	2.22	0.54
1:A:306:THR:O	1:A:309:ASN:HB3	2.08	0.54
1:B:223:LYS:HD3	1:B:225:ARG:HH21	1.70	0.54
1:C:35:GLY:O	1:C:36:ALA:O	2.25	0.54
1:C:55:ASN:O	1:C:59:ARG:HG3	2.07	0.54
1:A:141:VAL:HB	1:A:142:PRO:CD	2.38	0.54
1:B:232:TYR:CE1	1:B:242:LEU:HB2	2.43	0.54
1:B:317:TRP:CD2	1:B:458:GLY:HA3	2.42	0.54
1:C:325:VAL:HG21	1:C:406:MET:HE2	1.89	0.53
1:C:555:LYS:C	1:C:557:THR:H	2.17	0.53
1:A:210:ALA:HB3	1:A:223:LYS:HB2	1.89	0.53
1:A:317:TRP:CD2	1:A:458:GLY:HA3	2.44	0.53
1:B:88:ARG:HD3	1:B:263:GLY:O	2.07	0.53
1:C:36:ALA:HB1	1:C:45:SER:OG	2.09	0.53
1:A:395:GLN:O	1:A:398:THR:HG22	2.08	0.53
1:C:551:TRP:CZ3	1:C:587:ARG:HG3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:O	1:B:153:ILE:HG23	2.08	0.53
1:B:99:THR:HB	1:B:227:VAL:CG1	2.32	0.53
1:C:90:MET:HE2	1:C:264:PHE:CD2	2.44	0.53
1:B:325:VAL:HG21	1:B:406:MET:HE2	1.91	0.53
1:C:225:ARG:NH1	1:C:268:ARG:NH1	2.56	0.53
1:C:225:ARG:NH1	1:C:268:ARG:CZ	2.72	0.53
1:C:317:TRP:CD2	1:C:458:GLY:HA3	2.44	0.53
1:C:429:MET:O	1:C:432:ALA:HB3	2.09	0.53
1:B:160:MET:HE3	1:B:647:HIS:CB	2.36	0.53
1:C:662:MET:HB3	1:C:663:PRO:CD	2.39	0.53
1:A:301:THR:HG23	1:A:440:TRP:O	2.10	0.52
1:A:551:TRP:CZ3	1:A:587:ARG:HG3	2.44	0.52
1:C:94:PRO:HG3	1:C:269:ARG:NH1	2.24	0.52
1:B:33:LYS:HD2	1:B:34:GLU:H	1.75	0.52
1:B:43:LEU:HD12	1:B:44:LEU:N	2.24	0.52
1:B:301:THR:HG22	1:B:448:GLN:O	2.09	0.52
1:A:301:THR:HG22	1:A:448:GLN:O	2.08	0.52
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.44	0.52
1:A:325:VAL:HG21	1:A:406:MET:HE2	1.90	0.52
1:A:537:ARG:HH21	1:C:253:LYS:HZ2	1.58	0.52
1:B:600:ARG:HH11	1:B:600:ARG:HB3	1.75	0.52
1:C:94:PRO:CB	1:C:269:ARG:NH1	2.73	0.52
1:C:419:ALA:HB1	1:C:422:LEU:HD12	1.91	0.52
1:A:217:THR:CG2	1:A:219:LYS:HB2	2.40	0.52
1:A:364:PRO:CA	1:A:387:LEU:HD12	2.34	0.52
1:A:631:LYS:HE3	1:A:632:TRP:CZ2	2.45	0.52
1:C:599:SER:C	1:C:601:TYR:H	2.17	0.52
1:A:103:ALA:HB1	1:A:387:LEU:CD2	2.40	0.52
1:B:117:GLY:HA2	1:B:335:TRP:CD2	2.45	0.52
1:B:599:SER:OG	1:B:607:ARG:HG2	2.10	0.52
1:C:103:ALA:HB1	1:C:387:LEU:CD2	2.39	0.52
1:C:364:PRO:CA	1:C:387:LEU:HD12	2.34	0.52
1:A:43:LEU:HD12	1:A:44:LEU:N	2.25	0.52
1:C:210:ALA:HB3	1:C:223:LYS:HB2	1.91	0.52
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.92	0.52
1:B:506:ARG:O	1:B:507:ARG:C	2.53	0.51
1:A:232:TYR:CE1	1:A:242:LEU:HB2	2.46	0.51
1:A:555:LYS:C	1:A:557:THR:H	2.19	0.51
1:B:210:ALA:HB3	1:B:223:LYS:HB2	1.92	0.51
1:A:600:ARG:HH11	1:A:600:ARG:HB3	1.75	0.51
1:A:658:LEU:HG	1:A:662:MET:CE	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:TRP:CZ3	1:B:587:ARG:HG3	2.45	0.51
1:C:117:GLY:HA2	1:C:335:TRP:CD2	2.45	0.51
1:B:173:LYS:HB3	1:B:193:HIS:CE1	2.46	0.51
1:A:72:TYR:HB3	1:A:472:PHE:CZ	2.45	0.50
1:C:217:THR:C	1:C:219:LYS:H	2.19	0.50
1:B:72:TYR:CZ	1:B:476:LYS:HE2	2.46	0.50
1:B:564:TYR:CZ	1:B:568:LEU:CD1	2.94	0.50
1:C:88:ARG:HB2	1:C:211:ILE:HD12	1.94	0.50
1:C:658:LEU:HG	1:C:662:MET:CE	2.40	0.50
1:B:93:PHE:CD2	1:B:252:LEU:HD21	2.47	0.50
1:A:142:PRO:HG3	1:A:651:VAL:HG22	1.93	0.49
1:C:194:GLN:O	1:C:278:ALA:HB3	2.12	0.49
1:A:429:MET:O	1:A:432:ALA:HB3	2.12	0.49
1:C:631:LYS:HE3	1:C:632:TRP:CZ2	2.47	0.49
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.93	0.49
1:A:662:MET:HB3	1:A:663:PRO:CD	2.41	0.49
1:A:5:PRO:HD2	1:A:380:GLY:HA2	1.95	0.49
1:B:152:CYS:HA	1:B:156:PHE:CD1	2.47	0.49
1:B:201:VAL:HB	1:B:367:VAL:HA	1.93	0.49
1:B:141:VAL:HB	1:B:142:PRO:CD	2.43	0.49
1:B:337:ARG:HH11	1:B:362:LYS:HG2	1.75	0.49
1:B:419:ALA:HB1	1:B:422:LEU:HD12	1.94	0.49
1:C:152:CYS:HA	1:C:156:PHE:CD1	2.48	0.49
1:A:76:TYR:HA	1:A:502:LEU:HD12	1.95	0.49
1:C:141:VAL:HG21	1:C:288:GLN:HG3	1.94	0.49
1:C:217:THR:CG2	1:C:219:LYS:HB2	2.43	0.49
1:C:320:CYS:HB3	1:C:503:TYR:OH	2.13	0.49
1:C:600:ARG:HH11	1:C:600:ARG:HB3	1.76	0.49
1:B:225:ARG:NH1	1:B:268:ARG:CZ	2.76	0.49
1:C:144:LYS:HE3	1:C:642:HIS:CE1	2.48	0.49
1:A:95:MET:HE2	1:A:269:ARG:N	2.10	0.49
1:A:159:ASP:C	1:A:159:ASP:OD1	2.55	0.49
1:C:37:ILE:HG12	1:C:45:SER:HB3	1.94	0.49
1:C:281:ALA:HB3	1:C:282:PRO:HD3	1.94	0.49
1:C:301:THR:HG23	1:C:440:TRP:O	2.13	0.49
1:C:337:ARG:HH11	1:C:362:LYS:HG2	1.77	0.49
1:B:631:LYS:HE3	1:B:632:TRP:CZ2	2.48	0.48
1:A:195:MET:HE2	1:A:278:ALA:O	2.12	0.48
1:C:222:SER:HB2	1:C:247:LYS:HD2	1.94	0.48
1:A:307:ARG:HG2	1:A:499:ASP:OD2	2.13	0.48
1:B:429:MET:O	1:B:432:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ARG:O	1:C:507:ARG:C	2.56	0.48
1:A:290:VAL:HG11	1:A:400:LEU:HD13	1.96	0.48
1:B:217:THR:C	1:B:219:LYS:H	2.21	0.48
1:B:605:MET:HG2	1:B:606:ALA:O	2.13	0.48
1:A:225:ARG:NH1	1:A:268:ARG:CZ	2.77	0.48
1:C:104:SER:HA	1:C:388:GLU:HB2	1.95	0.48
1:C:418:THR:O	1:C:464:ALA:HA	2.14	0.48
1:B:68:ASN:N	1:B:68:ASN:HD22	2.11	0.48
1:B:138:LEU:HB2	1:B:662:MET:SD	2.54	0.48
1:B:153:ILE:HA	1:B:154:PRO:HA	1.63	0.48
1:C:522:LEU:HD21	1:C:571:ILE:HD11	1.95	0.48
1:A:37:ILE:HG12	1:A:45:SER:HB3	1.95	0.48
1:B:451:LYS:HD3	1:B:630:TYR:O	2.14	0.47
1:B:97:PRO:HB3	1:B:371:ALA:HB2	1.96	0.47
1:C:641:ILE:HD13	1:C:641:ILE:HA	1.74	0.47
1:A:46:VAL:HG12	1:A:90:MET:SD	2.55	0.47
1:A:228:ALA:HB1	1:A:232:TYR:HB3	1.95	0.47
1:B:526:PHE:C	1:B:528:PRO:HD3	2.39	0.47
1:B:555:LYS:C	1:B:557:THR:H	2.20	0.47
1:B:599:SER:CB	1:B:607:ARG:HA	2.44	0.47
1:C:95:MET:O	1:C:96:ILE:HG13	2.14	0.47
1:A:104:SER:HA	1:A:388:GLU:HB2	1.96	0.47
1:A:486:MET:HB2	1:A:488:ILE:HD11	1.96	0.47
1:B:217:THR:CG2	1:B:219:LYS:HB2	2.44	0.47
1:B:281:ALA:HB3	1:B:282:PRO:HD3	1.95	0.47
1:C:32:PHE:CD2	1:C:32:PHE:O	2.67	0.47
1:A:146:ARG:HD2	1:A:646:MET:SD	2.55	0.47
1:A:217:THR:C	1:A:219:LYS:H	2.23	0.47
1:C:286:VAL:HG21	1:C:353:TRP:CE2	2.49	0.47
1:C:564:TYR:CZ	1:C:568:LEU:CD1	2.98	0.47
1:B:599:SER:HB2	1:B:606:ALA:O	2.14	0.47
1:C:579:PHE:C	1:C:581:GLU:H	2.22	0.47
1:B:104:SER:HA	1:B:388:GLU:HB2	1.96	0.47
1:B:606:ALA:HB3	1:B:608:GLN:HE21	1.80	0.47
1:C:72:TYR:HB3	1:C:472:PHE:CZ	2.49	0.47
1:C:74:ARG:HH11	1:C:507:ARG:CB	2.27	0.47
1:C:93:PHE:HA	1:C:94:PRO:HD2	1.44	0.47
1:A:194:GLN:O	1:A:278:ALA:HB3	2.15	0.47
1:B:617:ILE:O	1:B:618:ASP:C	2.58	0.47
1:C:173:LYS:HB3	1:C:193:HIS:CE1	2.50	0.47
1:C:201:VAL:HB	1:C:367:VAL:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:HG22	1:A:219:LYS:HB2	1.97	0.47
1:B:288:GLN:HB3	1:B:289:PRO:HD3	1.96	0.47
1:C:141:VAL:HB	1:C:142:PRO:CD	2.45	0.47
1:A:90:MET:HE2	1:A:264:PHE:CD2	2.50	0.47
1:B:133:LEU:HD12	1:B:436:LEU:HD23	1.96	0.47
1:A:152:CYS:HA	1:A:156:PHE:CD1	2.50	0.46
1:A:201:VAL:HB	1:A:367:VAL:HA	1.97	0.46
1:B:228:ALA:HB1	1:B:232:TYR:HB3	1.97	0.46
1:A:631:LYS:HG2	1:A:632:TRP:CE2	2.50	0.46
1:B:225:ARG:NH1	1:B:268:ARG:NH1	2.64	0.46
1:A:68:ASN:N	1:A:68:ASN:HD22	2.13	0.46
1:B:222:SER:HB2	1:B:247:LYS:HD2	1.97	0.46
1:C:232:TYR:CE1	1:C:242:LEU:HB2	2.50	0.46
1:A:103:ALA:HB1	1:A:387:LEU:HD22	1.98	0.46
1:A:506:ARG:O	1:A:507:ARG:C	2.56	0.46
1:A:88:ARG:HB2	1:A:211:ILE:CD1	2.45	0.46
1:B:279:LEU:O	1:B:282:PRO:HD2	2.16	0.46
1:C:433:CYS:O	1:C:434:ARG:C	2.58	0.46
1:B:332:TRP:HA	1:B:333:PRO:HD3	1.81	0.46
1:B:403:THR:O	1:B:404:LEU:C	2.58	0.46
1:A:222:SER:HB2	1:A:247:LYS:HD2	1.97	0.46
1:B:522:LEU:HD21	1:B:571:ILE:HD11	1.97	0.46
1:B:608:GLN:O	1:B:610:GLY:N	2.49	0.46
1:A:26:GLN:O	1:A:30:ARG:HG3	2.16	0.46
1:A:153:ILE:HA	1:A:154:PRO:HA	1.64	0.46
1:B:433:CYS:O	1:B:434:ARG:C	2.57	0.46
1:C:363:LEU:HG	1:C:364:PRO:HD2	1.98	0.45
1:C:403:THR:O	1:C:404:LEU:C	2.59	0.45
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.79	0.45
1:A:403:THR:O	1:A:404:LEU:C	2.59	0.45
1:B:37:ILE:HG12	1:B:45:SER:HB3	1.97	0.45
1:B:202:VAL:CG1	1:B:272:ALA:HB3	2.47	0.45
1:B:290:VAL:HG11	1:B:400:LEU:HD13	1.99	0.45
1:B:579:PHE:C	1:B:581:GLU:H	2.25	0.45
1:B:364:PRO:HA	1:B:387:LEU:HD11	1.94	0.45
1:C:442:GLY:C	1:C:444:GLU:H	2.24	0.45
1:C:526:PHE:C	1:C:528:PRO:HD3	2.41	0.45
1:A:258:ILE:HG22	1:A:259:ASP:N	2.31	0.45
1:A:481:ASN:HA	1:A:482:PRO:HD3	1.70	0.45
1:C:160:MET:HE3	1:C:647:HIS:HB3	1.97	0.45
1:C:587:ARG:HD2	1:C:587:ARG:HA	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:GLN:HB2	1:B:609:ALA:H	1.47	0.45
1:C:46:VAL:HA	1:C:51:LEU:HD21	1.98	0.45
1:A:143:LEU:HB2	1:A:654:THR:HG21	1.98	0.45
1:A:564:TYR:CZ	1:A:568:LEU:CD1	3.00	0.45
1:B:517:ASN:HB3	1:B:520:SER:OG	2.17	0.45
1:A:250:SER:C	1:A:252:LEU:N	2.73	0.45
1:A:518:ILE:HD12	1:A:518:ILE:HA	1.81	0.45
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.51	0.45
1:A:99:THR:HG22	1:A:271:THR:CG2	2.47	0.45
1:B:101:PRO:O	1:B:233:ALA:HB1	2.17	0.45
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.79	0.45
1:C:311:GLU:HG2	1:C:315:LYS:HE2	1.99	0.45
1:C:557:THR:HG22	1:C:558:TYR:CG	2.52	0.45
1:A:526:PHE:C	1:A:528:PRO:HD3	2.42	0.45
1:A:579:PHE:C	1:A:581:GLU:H	2.25	0.45
1:B:658:LEU:HG	1:B:662:MET:CE	2.45	0.45
1:C:573:ARG:O	1:C:576:TRP:HB2	2.17	0.45
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.99	0.44
1:B:90:MET:O	1:B:91:ASN:C	2.61	0.44
1:B:216:LYS:HE3	1:B:216:LYS:HB3	1.74	0.44
1:B:564:TYR:CZ	1:B:568:LEU:HD11	2.52	0.44
1:A:46:VAL:HA	1:A:51:LEU:HD21	1.99	0.44
1:B:46:VAL:HA	1:B:51:LEU:HD21	1.99	0.44
1:B:141:VAL:HG11	1:B:292:ASN:ND2	2.32	0.44
1:B:339:LEU:HD23	1:B:339:LEU:C	2.42	0.44
1:A:225:ARG:NH1	1:A:268:ARG:NH1	2.65	0.44
1:B:175:GLU:HA	1:B:352:TRP:CD2	2.52	0.44
1:C:68:ASN:N	1:C:68:ASN:HD22	2.15	0.44
1:C:228:ALA:HB1	1:C:232:TYR:HB3	1.99	0.44
1:C:159:ASP:C	1:C:159:ASP:OD1	2.61	0.44
1:C:222:SER:HB3	1:C:265:PHE:CD2	2.53	0.44
1:C:598:LEU:O	1:C:601:TYR:HB2	2.17	0.44
1:A:311:GLU:HG2	1:A:315:LYS:HE2	2.00	0.44
1:A:540:SER:HB2	1:A:644:VAL:O	2.18	0.44
1:B:463:ARG:O	1:B:466:VAL:HG12	2.18	0.44
1:C:43:LEU:HD12	1:C:43:LEU:C	2.43	0.44
1:B:573:ARG:O	1:B:576:TRP:HB2	2.18	0.44
1:C:508:GLU:HA	1:C:509:PRO:HD3	1.85	0.44
1:A:555:LYS:HE2	1:A:555:LYS:HB2	1.87	0.43
1:C:16:MET:HE2	1:C:16:MET:HB3	1.79	0.43
1:A:16:MET:HE2	1:A:16:MET:HB3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD13	1:A:411:LEU:CD2	2.48	0.43
1:B:631:LYS:HG2	1:B:632:TRP:CE2	2.53	0.43
1:C:410:TYR:O	1:C:411:LEU:C	2.61	0.43
1:B:217:THR:HG22	1:B:219:LYS:HB2	2.00	0.43
1:B:379:LEU:O	1:B:387:LEU:HD11	2.17	0.43
1:C:303:HIS:CD2	1:C:305:THR:HG23	2.53	0.43
1:A:418:THR:O	1:A:464:ALA:HA	2.18	0.43
1:C:345:LEU:HD23	1:C:345:LEU:HA	1.88	0.43
1:C:517:ASN:OD1	1:C:519:ASN:N	2.52	0.43
1:A:173:LYS:HB3	1:A:193:HIS:CE1	2.53	0.43
1:A:405:LEU:HG	1:A:406:MET:N	2.32	0.43
1:B:16:MET:HE2	1:B:16:MET:HB3	1.83	0.43
1:B:102:LEU:HD12	1:B:233:ALA:HA	2.00	0.43
1:C:7:PHE:HA	1:C:8:PRO:HD3	1.85	0.43
1:C:217:THR:HG22	1:C:219:LYS:HB2	2.00	0.43
1:C:336:LEU:HD21	1:C:404:LEU:HD12	2.00	0.43
1:C:481:ASN:HA	1:C:482:PRO:HD3	1.67	0.43
1:B:504:ASP:CG	1:B:505:SER:N	2.76	0.43
1:B:611:LEU:O	1:B:612:ALA:C	2.62	0.43
1:C:232:TYR:CE2	1:C:237:GLY:HA2	2.54	0.43
1:A:573:ARG:O	1:A:576:TRP:HB2	2.19	0.43
1:A:522:LEU:HD21	1:A:571:ILE:HD11	1.99	0.43
1:C:182:LEU:HD21	1:C:355:LYS:HB2	2.01	0.43
1:C:405:LEU:HG	1:C:406:MET:N	2.31	0.43
1:B:144:LYS:HA	1:B:648:GLY:HA2	2.01	0.42
1:B:518:ILE:HD12	1:B:518:ILE:HA	1.89	0.42
1:B:641:ILE:HD13	1:B:641:ILE:HA	1.74	0.42
1:C:133:LEU:O	1:C:293:LYS:HE2	2.19	0.42
1:C:290:VAL:HG11	1:C:400:LEU:HD13	2.01	0.42
1:C:631:LYS:HG2	1:C:632:TRP:CE2	2.54	0.42
1:A:617:ILE:O	1:A:618:ASP:C	2.62	0.42
1:B:55:ASN:O	1:B:59:ARG:HG3	2.18	0.42
1:B:225:ARG:HD2	1:B:268:ARG:HD2	2.01	0.42
1:B:363:LEU:HG	1:B:364:PRO:HD2	2.01	0.42
1:C:153:ILE:HA	1:C:154:PRO:HA	1.61	0.42
1:C:451:LYS:HD3	1:C:630:TYR:O	2.18	0.42
1:B:320:CYS:HB3	1:B:503:TYR:OH	2.19	0.42
1:C:372:PRO:O	1:C:373:GLU:HB2	2.17	0.42
1:A:85:PHE:O	1:A:211:ILE:HD12	2.18	0.42
1:B:250:SER:C	1:B:252:LEU:N	2.75	0.42
1:B:429:MET:HB2	1:B:430:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.80	0.42
1:C:22:ILE:H	1:C:22:ILE:HG12	1.63	0.42
1:B:311:GLU:HG2	1:B:315:LYS:HE2	2.01	0.42
1:A:102:LEU:HD12	1:A:233:ALA:HA	2.00	0.42
1:A:372:PRO:O	1:A:373:GLU:HB2	2.20	0.42
1:A:463:ARG:O	1:A:466:VAL:HG12	2.19	0.42
1:B:280:ASN:ND2	1:B:396:GLY:H	2.17	0.42
1:C:37:ILE:HG23	1:C:92:GLY:HA3	2.01	0.42
1:C:449:ILE:O	1:C:449:ILE:HG13	2.20	0.42
1:A:175:GLU:HA	1:A:352:TRP:CD2	2.55	0.42
1:A:303:HIS:HE2	1:A:305:THR:CG2	2.33	0.42
1:A:317:TRP:CE3	1:A:458:GLY:HA3	2.55	0.42
1:A:404:LEU:C	1:A:404:LEU:HD13	2.44	0.42
1:A:419:ALA:HB1	1:A:422:LEU:HD12	2.00	0.42
1:B:508:GLU:HA	1:B:509:PRO:HD3	1.87	0.42
1:C:463:ARG:O	1:C:466:VAL:HG12	2.20	0.42
1:C:624:ASP:OD1	1:C:626:ASN:HB2	2.20	0.42
1:A:160:MET:CE	1:A:647:HIS:HB3	2.40	0.42
1:B:90:MET:HE2	1:B:264:PHE:CB	2.49	0.42
1:B:393:SER:O	1:B:398:THR:HG21	2.19	0.42
1:B:606:ALA:CB	1:B:608:GLN:HE21	2.33	0.42
1:C:555:LYS:HE2	1:C:555:LYS:HB2	1.89	0.42
1:C:650:SER:OG	1:C:653:LYS:HD2	2.20	0.42
1:A:143:LEU:H	1:A:654:THR:HG21	1.85	0.42
1:A:320:CYS:HB3	1:A:503:TYR:OH	2.19	0.42
1:A:587:ARG:HD2	1:A:587:ARG:HA	1.73	0.42
1:A:611:LEU:O	1:A:612:ALA:C	2.62	0.42
1:C:486:MET:HB2	1:C:488:ILE:HD11	2.02	0.42
1:A:43:LEU:HD12	1:A:43:LEU:C	2.45	0.41
1:B:94:PRO:C	1:B:266:CYS:HB3	2.45	0.41
1:B:522:LEU:CD2	1:B:571:ILE:HD11	2.50	0.41
1:A:112:ALA:O	1:A:113:ASP:HB2	2.19	0.41
1:A:433:CYS:O	1:A:434:ARG:C	2.62	0.41
1:C:599:SER:C	1:C:601:TYR:N	2.78	0.41
1:A:72:TYR:CE1	1:A:476:LYS:HE2	2.53	0.41
1:A:144:LYS:HA	1:A:648:GLY:HA2	2.01	0.41
1:A:537:ARG:CZ	1:C:253:LYS:HE3	2.50	0.41
1:C:617:ILE:O	1:C:618:ASP:C	2.63	0.41
1:A:7:PHE:HA	1:A:8:PRO:HD3	1.87	0.41
1:A:160:MET:O	1:A:164:ILE:HG12	2.20	0.41
1:A:429:MET:HB2	1:A:430:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:TRP:CE3	1:A:587:ARG:HG3	2.55	0.41
1:B:182:LEU:HD21	1:B:355:LYS:HB2	2.01	0.41
1:B:537:ARG:HH11	1:B:537:ARG:HD3	1.65	0.41
1:B:557:THR:HG22	1:B:558:TYR:CG	2.55	0.41
1:C:96:ILE:HA	1:C:97:PRO:HA	1.81	0.41
1:A:90:MET:HE2	1:A:264:PHE:CG	2.56	0.41
1:A:319:LEU:HD12	1:A:320:CYS:H	1.86	0.41
1:A:442:GLY:C	1:A:444:GLU:H	2.27	0.41
1:A:557:THR:HG22	1:A:558:TYR:CG	2.55	0.41
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.85	0.41
1:B:527:SER:N	1:B:528:PRO:HD3	2.35	0.41
1:A:143:LEU:N	1:A:654:THR:HG21	2.36	0.41
1:A:229:ASP:O	1:A:230:PHE:C	2.63	0.41
1:A:286:VAL:HG21	1:A:353:TRP:CE2	2.56	0.41
1:A:429:MET:CB	1:A:430:PRO:HD3	2.50	0.41
1:A:641:ILE:HD13	1:A:641:ILE:HA	1.71	0.41
1:C:95:MET:HE2	1:C:269:ARG:N	2.18	0.41
1:A:290:VAL:CG1	1:A:400:LEU:HD13	2.51	0.41
1:B:418:THR:O	1:B:464:ALA:HA	2.21	0.41
1:A:143:LEU:HB2	1:A:654:THR:CG2	2.50	0.41
1:B:31:SER:O	1:B:32:PHE:C	2.64	0.41
1:B:91:ASN:HA	1:B:267:GLU:OE1	2.21	0.41
1:B:300:TYR:CD1	1:B:442:GLY:HA3	2.56	0.41
1:A:279:LEU:O	1:A:282:PRO:HD2	2.21	0.41
1:A:308:LEU:HA	1:A:308:LEU:HD12	1.84	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.88	0.41
1:A:504:ASP:CG	1:A:505:SER:N	2.78	0.41
1:B:152:CYS:HA	1:B:156:PHE:CE1	2.56	0.41
1:B:429:MET:CB	1:B:430:PRO:HD3	2.51	0.41
1:C:5:PRO:HD2	1:C:380:GLY:HA2	2.03	0.41
1:C:74:ARG:NH1	1:C:507:ARG:CB	2.83	0.41
1:A:127:PHE:CE2	1:A:408:ILE:HB	2.56	0.41
1:B:94:PRO:CB	1:B:269:ARG:HG3	2.51	0.41
1:C:32:PHE:CD2	1:C:372:PRO:HG3	2.56	0.41
1:A:379:LEU:O	1:A:387:LEU:HD11	2.21	0.40
1:B:317:TRP:CE3	1:B:458:GLY:HA3	2.56	0.40
1:B:380:GLY:O	1:B:382:PRO:HD3	2.21	0.40
1:C:216:LYS:HE3	1:C:216:LYS:HB3	1.72	0.40
1:C:286:VAL:C	1:C:289:PRO:HD2	2.46	0.40
1:C:429:MET:HB2	1:C:430:PRO:HD3	2.03	0.40
1:C:429:MET:CB	1:C:430:PRO:HD3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:HB3	1:A:216:LYS:HE3	1.67	0.40
1:C:112:ALA:O	1:C:113:ASP:HB2	2.21	0.40
1:C:408:ILE:O	1:C:412:VAL:HG23	2.20	0.40
1:A:449:ILE:O	1:A:449:ILE:HG13	2.20	0.40
1:B:4:ALA:HA	1:B:5:PRO:HD3	1.90	0.40
1:B:85:PHE:O	1:B:211:ILE:HD12	2.21	0.40
1:B:159:ASP:OD1	1:B:159:ASP:C	2.63	0.40
1:C:300:TYR:CD1	1:C:442:GLY:HA3	2.56	0.40
1:A:3:ARG:NH2	1:A:231:GLU:OE2	2.54	0.40
1:B:43:LEU:HD12	1:B:43:LEU:C	2.47	0.40
1:B:408:ILE:O	1:B:412:VAL:HG23	2.21	0.40
1:C:131:VAL:HG21	1:C:340:ILE:HA	2.03	0.40
1:C:250:SER:C	1:C:252:LEU:N	2.79	0.40
1:C:522:LEU:CD2	1:C:571:ILE:HD11	2.50	0.40

All (2) 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:506:ARG:NH2	1:C:445:GLU:N[3_544]	2.01	0.19
1:A:240:GLY:N	1:C:217:THR:O[2_554]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	650/664 (98%)	589 (91%)	59 (9%)	2 (0%)	36	68
1	B	659/664 (99%)	586 (89%)	68 (10%)	5 (1%)	16	50
1	C	650/664 (98%)	575 (88%)	68 (10%)	7 (1%)	11	43
All	All	1959/1992 (98%)	1750 (89%)	195 (10%)	14 (1%)	18	52

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	609	ALA
1	C	36	ALA
1	B	610	GLY
1	C	630	TYR
1	A	630	TYR
1	B	630	TYR
1	C	581	GLU
1	A	581	GLU
1	B	581	GLU
1	C	95	MET
1	C	507	ARG
1	C	529	GLU
1	B	91	ASN
1	C	32	PHE

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	550/557 (99%)	522 (95%)	28 (5%)	21	54
1	B	554/557 (100%)	519 (94%)	35 (6%)	16	48
1	C	550/557 (99%)	520 (94%)	30 (6%)	19	52
All	All	1654/1671 (99%)	1561 (94%)	93 (6%)	19	52

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	31	SER
1	A	44	LEU
1	A	55	ASN
1	A	208	THR
1	A	234	VAL
1	A	259	ASP

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Mol	Chain	Res	Type
1	A	271	THR
1	A	308	LEU
1	A	363	LEU
1	A	365	VAL
1	A	392	SER
1	A	404	LEU
1	A	445	GLU
1	A	466	VAL
1	A	497	LEU
1	A	518	ILE
1	A	529	GLU
1	A	556	ASP
1	A	557	THR
1	A	576	TRP
1	A	582	SER
1	A	587	ARG
1	A	589	ASP
1	A	611	LEU
1	A	615	THR
1	A	626	ASN
1	A	641	ILE
1	B	22	ILE
1	B	31	SER
1	B	44	LEU
1	B	68	ASN
1	B	91	ASN
1	B	143	LEU
1	B	202	VAL
1	B	208	THR
1	B	234	VAL
1	B	259	ASP
1	B	271	THR
1	B	308	LEU
1	B	363	LEU
1	B	365	VAL
1	B	392	SER
1	B	404	LEU
1	B	445	GLU
1	B	466	VAL
1	B	497	LEU
1	B	500	ILE
1	B	518	ILE

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Mol	Chain	Res	Type
1	B	529	GLU
1	B	537	ARG
1	B	556	ASP
1	B	557	THR
1	B	576	TRP
1	B	582	SER
1	B	587	ARG
1	B	589	ASP
1	B	608	GLN
1	B	611	LEU
1	B	615	THR
1	B	626	ASN
1	B	628	LEU
1	B	641	ILE
1	C	22	ILE
1	C	44	LEU
1	C	46	VAL
1	C	55	ASN
1	C	91	ASN
1	C	143	LEU
1	C	208	THR
1	C	227	VAL
1	C	234	VAL
1	C	259	ASP
1	C	271	THR
1	C	308	LEU
1	C	363	LEU
1	C	392	SER
1	C	404	LEU
1	C	445	GLU
1	C	466	VAL
1	C	497	LEU
1	C	518	ILE
1	C	529	GLU
1	C	556	ASP
1	C	557	THR
1	C	576	TRP
1	C	582	SER
1	C	587	ARG
1	C	589	ASP
1	C	611	LEU
1	C	615	THR

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Mol	Chain	Res	Type
1	C	626	ASN
1	C	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	64	HIS
1	A	191	GLN
1	A	443	HIS
1	A	626	ASN
1	B	15	GLN
1	B	25	GLN
1	B	64	HIS
1	B	191	GLN
1	B	193	HIS
1	B	443	HIS
1	B	608	GLN
1	B	626	ASN
1	C	15	GLN
1	C	25	GLN
1	C	55	ASN
1	C	64	HIS
1	C	191	GLN
1	C	280	ASN
1	C	443	HIS
1	C	626	ASN

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	654/664 (98%)	0.02	7 (1%) 78 61	9, 32, 66, 101	0
1	B	661/664 (99%)	-0.02	6 (0%) 81 64	9, 33, 68, 118	0
1	C	654/664 (98%)	0.30	27 (4%) 41 25	12, 38, 72, 132	0
All	All	1969/1992 (98%)	0.10	40 (2%) 65 45	9, 34, 69, 132	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	GLY	3.9
1	B	608	GLN	3.7
1	B	606	ALA	3.3
1	C	258	ILE	3.0
1	A	240	GLY	2.8
1	B	214	ASP	2.8
1	C	252	LEU	2.8
1	C	257	GLY	2.6
1	C	603	ALA	2.6
1	C	249	ALA	2.6
1	A	259	ASP	2.6
1	C	211	ILE	2.5
1	C	213	LEU	2.5
1	B	613	GLU	2.5
1	A	576	TRP	2.5
1	C	586	TYR	2.5
1	A	264	PHE	2.4
1	A	506	ARG	2.4
1	C	576	TRP	2.3
1	C	215	PRO	2.3
1	C	579	PHE	2.2
1	A	70	ASP	2.2
1	C	209	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	264	PHE	2.2
1	C	216	LYS	2.2
1	C	259	ASP	2.2
1	B	607	ARG	2.2
1	C	217	THR	2.1
1	C	594	ASP	2.1
1	C	73	GLY	2.1
1	C	531	GLY	2.1
1	A	635	ALA	2.1
1	C	260	VAL	2.1
1	B	603	ALA	2.1
1	C	56	GLU	2.1
1	C	536	VAL	2.1
1	C	639	ALA	2.1
1	C	533	GLN	2.1
1	C	214	ASP	2.0
1	C	93	PHE	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	MN	A	1664	1/1	0.96	0.04	59,59,59,59	0
2	MN	B	1664	1/1	0.97	0.05	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.