



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:29 PM UTC

PDB ID : 1NB4 / pdb_00001nb4
Title : HC-J4 RNA polymerase apo-form
Authors : Jaeger, J.; O'Farrell, D.J.; Trowbridge, R.; Rowlands, D.J.
Deposited on : 2002-12-02
Resolution : 2.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

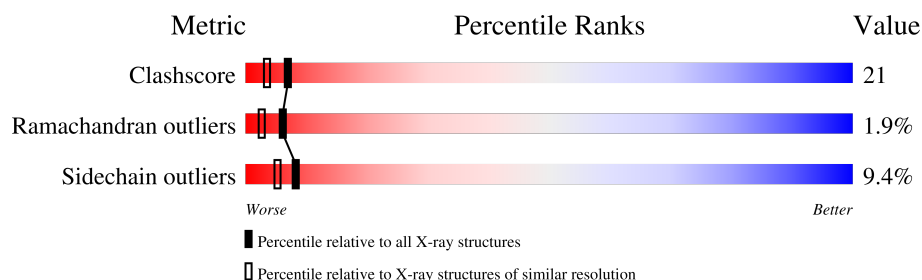
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	570	 64% 30% 5% ..
1	B	570	 64% 25% 9% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9554 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 polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4388	2763	777	816	32			
1	B	565	Total	C	N	O	S	0	0	0
			4383	2760	776	815	32			

- Molecule 2 is water.

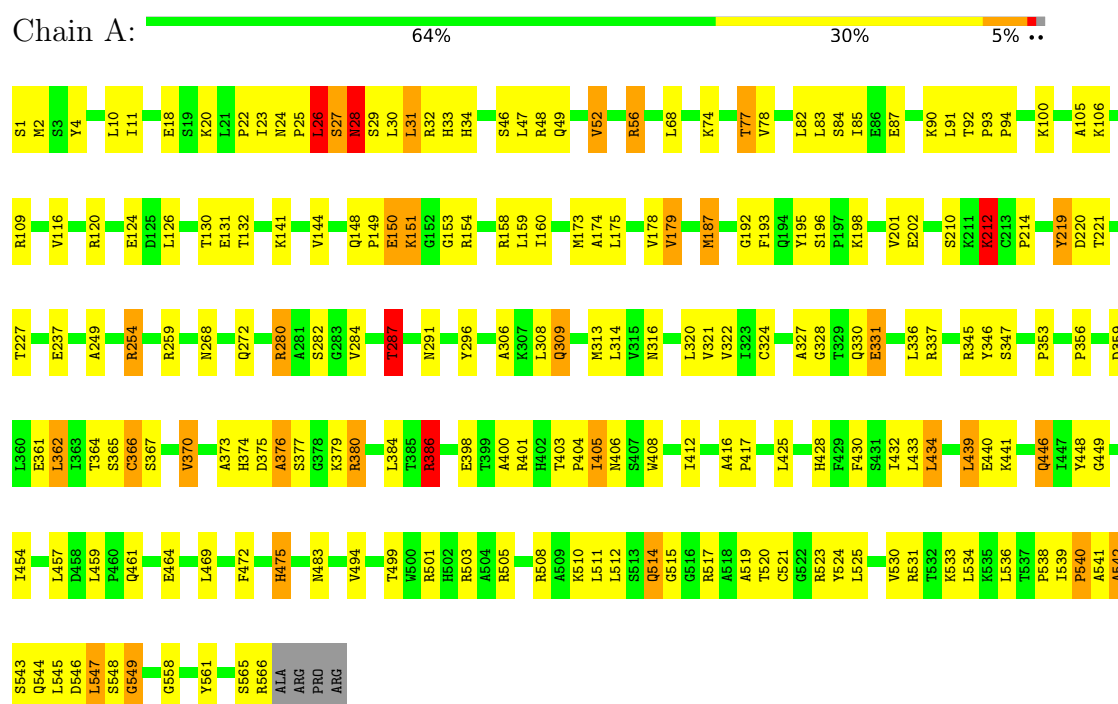
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	344	Total	O	0	0
			344	344		
2	B	439	Total	O	0	0
			439	439		

3 Residue-property plots

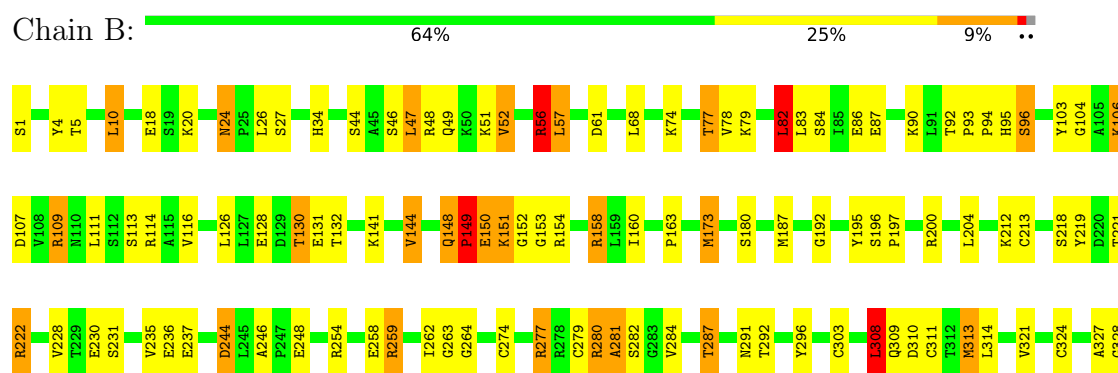
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

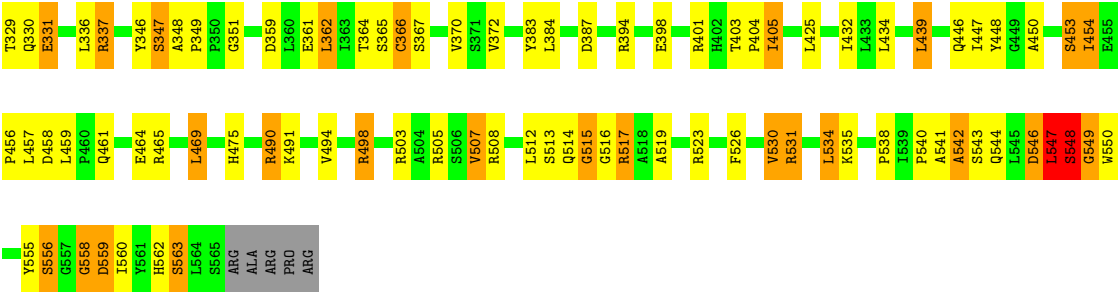
Note EDS was not executed.

- Molecule 1: polypeptide



- Molecule 1: polypeptide





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.69Å 108.71Å 135.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.3 (55.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9554	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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	1.04	2/4484 (0.0%)	1.26	38/6087 (0.6%)
1	B	1.17	9/4479 (0.2%)	1.27	42/6080 (0.7%)
All	All	1.11	11/8963 (0.1%)	1.27	80/12167 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	PRO	CA-C	8.19	1.57	1.52
1	B	173	MET	SD-CE	-7.41	1.61	1.79
1	B	450	ALA	CA-CB	-7.36	1.42	1.53
1	A	91	LEU	CA-C	6.34	1.61	1.52
1	A	2	MET	SD-CE	-5.86	1.65	1.79
1	B	246	ALA	CA-CB	-5.31	1.44	1.53
1	B	230	GLU	CA-C	5.29	1.59	1.52
1	B	231	SER	CA-C	5.23	1.59	1.52
1	B	494	VAL	CA-C	5.05	1.58	1.52
1	B	292	THR	C-O	5.05	1.29	1.24
1	B	347	SER	CA-C	5.00	1.59	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	ASP	N-CA-C	9.11	120.80	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	THR	CA-C-N	-8.98	111.13	120.38
1	A	92	THR	C-N-CA	-8.98	111.13	120.38
1	B	558	GLY	N-CA-C	-8.56	99.41	112.51
1	A	196	SER	N-CA-C	-7.70	98.83	110.07
1	A	287	THR	N-CA-C	7.67	120.72	111.82
1	B	475	HIS	N-CA-C	7.50	126.78	110.80
1	B	366	CYS	N-CA-C	-7.47	102.68	112.24
1	A	475	HIS	CA-C-N	-7.23	113.23	123.20
1	A	475	HIS	C-N-CA	-7.23	113.23	123.20
1	A	78	VAL	N-CA-C	7.14	118.93	109.21
1	B	196	SER	N-CA-C	-6.98	99.88	110.07
1	A	219	TYR	CA-C-N	-6.75	113.48	122.99
1	A	219	TYR	C-N-CA	-6.75	113.48	122.99
1	A	11	ILE	N-CA-C	-6.69	98.00	108.23
1	B	218	SER	N-CA-C	-6.67	99.35	109.95
1	B	78	VAL	N-CA-C	6.66	118.99	108.87
1	B	387	ASP	CA-C-N	-6.56	113.39	121.00
1	B	387	ASP	C-N-CA	-6.56	113.39	121.00
1	A	214	PRO	N-CA-C	6.51	121.72	111.38
1	B	113	SER	N-CA-C	6.47	117.99	111.07
1	B	131	GLU	N-CA-C	6.38	121.66	113.18
1	B	192	GLY	N-CA-C	6.24	121.41	113.24
1	A	131	GLU	N-CA-C	6.18	123.96	110.80
1	B	526	PHE	N-CA-C	6.16	120.10	112.59
1	A	193	PHE	N-CA-C	6.14	120.38	113.01
1	A	475	HIS	N-CA-C	6.12	123.84	110.80
1	A	366	CYS	N-CA-C	-6.08	105.16	112.58
1	B	548	SER	N-CA-C	-5.91	98.21	110.80
1	B	213	CYS	CA-C-N	5.87	125.83	119.78
1	B	213	CYS	C-N-CA	5.87	125.83	119.78
1	A	337	ARG	N-CA-C	-5.85	104.08	111.11
1	A	10	LEU	N-CA-C	5.69	118.23	110.55
1	A	175	LEU	N-CA-C	5.67	122.84	113.89
1	B	507	VAL	CB-CA-C	-5.67	104.40	112.22
1	A	558	GLY	N-CA-C	5.65	124.71	115.73
1	B	56	ARG	CG-CD-NE	-5.63	99.61	112.00
1	A	280	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	B	309	GLN	N-CA-C	5.56	118.02	109.07
1	A	405	ILE	N-CA-C	5.56	115.95	108.17
1	B	530	VAL	N-CA-C	5.55	117.17	109.45
1	A	195	TYR	N-CA-C	5.55	118.53	109.59
1	B	324	CYS	N-CA-C	5.54	115.59	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	TYR	N-CA-C	5.53	118.82	109.76
1	B	128	GLU	N-CA-C	5.52	120.12	112.45
1	A	100	LYS	N-CA-C	-5.48	106.43	113.01
1	A	370	VAL	CB-CA-C	-5.47	103.71	111.21
1	B	559	ASP	N-CA-C	-5.47	99.15	110.80
1	A	192	GLY	N-CA-C	5.46	119.28	112.73
1	A	28	ASN	N-CA-C	-5.42	105.48	111.71
1	A	174	ALA	N-CA-C	5.38	119.01	112.23
1	A	212	LYS	N-CA-C	-5.37	105.34	111.14
1	B	280	ARG	NE-CZ-NH2	-5.35	114.38	119.20
1	B	95	HIS	N-CA-C	5.34	118.81	112.72
1	B	348	ALA	CA-C-N	5.32	123.49	119.66
1	B	348	ALA	C-N-CA	5.32	123.49	119.66
1	B	329	THR	N-CA-C	5.31	116.76	110.97
1	B	372	VAL	CB-CA-C	-5.26	102.78	110.62
1	A	309	GLN	N-CA-C	5.26	118.13	109.76
1	B	372	VAL	N-CA-C	5.26	116.06	108.48
1	B	498	ARG	CG-CD-NE	5.25	123.55	112.00
1	A	521	CYS	N-CA-C	-5.22	105.67	111.36
1	B	82	LEU	N-CA-C	-5.20	102.05	110.32
1	A	386	ARG	CG-CD-NE	-5.19	100.59	112.00
1	A	549	GLY	N-CA-C	-5.17	106.94	114.90
1	A	254	ARG	CG-CD-NE	-5.17	100.63	112.00
1	B	235	VAL	N-CA-C	-5.16	105.51	110.72
1	B	560	ILE	N-CA-C	5.16	115.39	108.17
1	A	449	GLY	N-CA-C	5.13	121.19	115.08
1	B	219	TYR	CA-C-N	-5.13	115.77	123.00
1	B	219	TYR	C-N-CA	-5.13	115.77	123.00
1	A	27	SER	N-CA-C	-5.12	105.88	111.82
1	A	406	ASN	N-CA-C	5.11	117.49	107.57
1	A	187	MET	N-CA-C	5.10	119.60	113.17
1	B	244	ASP	N-CA-C	-5.10	101.44	109.25
1	B	281	ALA	N-CA-C	-5.10	102.14	110.20
1	B	432	ILE	CB-CA-C	-5.08	105.31	111.87
1	A	446	GLN	N-CA-C	5.08	117.72	109.24
1	B	308	LEU	N-CA-C	-5.05	102.90	110.23
1	B	469	LEU	N-CA-C	5.00	118.15	111.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	TYR	Sidechain
1	B	383	TYR	Sidechain
1	B	498	ARG	Sidechain

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	4388	0	4383	192	0
1	B	4383	0	4381	179	0
2	A	344	0	0	35	0
2	B	439	0	0	43	0
All	All	9554	0	8764	370	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 21.

All (370) 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:130:THR:HB	2:B:800:HOH:O	1.31	1.25
1:B:277:ARG:HH11	1:B:277:ARG:HB3	1.14	1.10
1:A:547:LEU:HD12	1:A:565:SER:H	1.06	1.08
1:B:109:ARG:NH1	1:B:109:ARG:HB2	1.72	1.05
1:A:327:ALA:O	1:A:331:GLU:HG3	1.61	1.01
1:A:20:LYS:O	1:A:22:PRO:HD3	1.65	0.97
1:B:277:ARG:HH11	1:B:277:ARG:CB	1.77	0.96
1:A:373:ALA:HB1	2:A:872:HOH:O	1.66	0.95
1:B:461:GLN:HB3	1:B:542:ALA:HA	1.49	0.94
1:B:337:ARG:HG3	2:B:977:HOH:O	1.67	0.94
1:A:24:ASN:ND2	1:A:27:SER:H	1.66	0.93
1:B:200:ARG:NH1	1:B:204:LEU:HD11	1.83	0.93
1:B:200:ARG:NE	2:B:749:HOH:O	2.01	0.92
1:A:405:ILE:HD11	1:A:446:GLN:HG2	1.49	0.92
1:B:61:ASP:CG	2:B:588:HOH:O	2.17	0.87
1:A:56:ARG:NH2	2:A:643:HOH:O	2.08	0.87
1:A:56:ARG:NE	2:A:643:HOH:O	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HD12	1:A:565:SER:N	1.90	0.87
1:B:277:ARG:CZ	2:B:628:HOH:O	2.21	0.87
1:B:277:ARG:HB3	1:B:277:ARG:NH1	1.88	0.86
1:A:24:ASN:ND2	1:A:27:SER:N	2.24	0.86
1:A:141:LYS:HE3	1:A:158:ARG:NH2	1.89	0.86
1:B:200:ARG:CZ	2:B:749:HOH:O	2.24	0.85
1:A:84:SER:OG	1:A:87:GLU:HG3	1.76	0.85
1:A:24:ASN:HD22	1:A:27:SER:HB2	1.40	0.84
1:B:327:ALA:O	1:B:331:GLU:HG3	1.77	0.84
1:B:264:GLY:N	1:B:277:ARG:HH12	1.76	0.84
1:A:124:GLU:HG3	2:A:881:HOH:O	1.77	0.83
1:A:547:LEU:CD1	1:A:565:SER:H	1.91	0.82
1:A:105:ALA:O	1:A:109:ARG:HG3	1.80	0.81
1:A:148:GLN:HG2	1:A:150:GLU:H	1.45	0.81
1:B:18:GLU:HG2	1:B:401:ARG:NH1	1.95	0.81
1:A:56:ARG:HB2	1:A:56:ARG:NH1	1.95	0.80
1:B:141:LYS:NZ	1:B:158:ARG:HH12	1.81	0.79
1:B:464:GLU:HG3	1:B:469:LEU:HD12	1.63	0.79
1:B:222:ARG:HG3	1:B:351:GLY:HA2	1.65	0.79
1:A:24:ASN:HD22	1:A:27:SER:CB	1.95	0.78
1:A:56:ARG:HB2	1:A:56:ARG:HH11	1.49	0.78
1:B:109:ARG:HB2	1:B:109:ARG:HH11	1.46	0.78
1:A:268:ASN:HD21	1:A:272:GLN:HE21	1.29	0.77
1:A:56:ARG:CZ	2:A:643:HOH:O	2.30	0.76
1:B:18:GLU:HG2	1:B:401:ARG:CZ	2.15	0.76
1:B:148:GLN:HE21	1:B:153:GLY:HA3	1.49	0.75
1:B:132:THR:O	1:B:259:ARG:CD	2.34	0.75
1:A:280:ARG:HD2	1:A:291:ASN:OD1	1.87	0.74
1:A:359:ASP:HB3	1:A:362:LEU:HD22	1.68	0.74
1:B:160:ILE:HD12	1:B:282:SER:OG	1.87	0.74
1:A:154:ARG:HG3	1:A:154:ARG:HH11	1.53	0.74
1:B:403:THR:HB	1:B:404:PRO:HD2	1.69	0.74
1:B:109:ARG:HH11	1:B:109:ARG:CB	2.01	0.74
1:B:132:THR:O	1:B:259:ARG:HD2	1.88	0.73
1:A:22:PRO:HB2	2:A:619:HOH:O	1.88	0.73
1:A:475:HIS:N	2:A:872:HOH:O	2.20	0.73
1:A:148:GLN:CD	1:A:150:GLU:HG2	2.12	0.73
1:A:132:THR:O	1:A:259:ARG:HD2	1.88	0.73
1:B:548:SER:O	1:B:550:TRP:N	2.22	0.73
1:A:24:ASN:HD22	1:A:27:SER:N	1.84	0.72
1:B:558:GLY:O	2:B:591:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLY:HA2	2:B:644:HOH:O	1.88	0.72
1:A:28:ASN:HB2	2:A:774:HOH:O	1.90	0.72
1:B:361:GLU:HB2	2:B:948:HOH:O	1.90	0.72
1:A:198:LYS:O	1:A:201:VAL:HG12	1.90	0.71
1:A:132:THR:O	1:A:259:ARG:CD	2.38	0.71
1:B:277:ARG:NE	2:B:628:HOH:O	2.21	0.70
1:A:26:LEU:O	1:A:29:SER:HB3	1.90	0.70
1:A:148:GLN:OE1	1:A:153:GLY:HA3	1.89	0.70
1:B:154:ARG:HD3	2:B:958:HOH:O	1.91	0.70
1:B:303:CYS:SG	1:B:313:MET:HE1	2.30	0.70
1:B:130:THR:HG21	2:B:680:HOH:O	1.92	0.70
1:B:490:ARG:HE	1:B:490:ARG:HA	1.57	0.70
1:B:534:LEU:HD12	1:B:535:LYS:N	2.07	0.70
1:B:465:ARG:HD3	1:B:543:SER:HA	1.74	0.69
1:A:178:VAL:HG23	2:A:649:HOH:O	1.92	0.69
1:A:24:ASN:HD22	1:A:27:SER:H	1.36	0.69
1:B:200:ARG:HH12	1:B:204:LEU:HD11	1.56	0.69
1:A:501:ARG:HB3	2:A:794:HOH:O	1.92	0.69
1:B:534:LEU:HD12	1:B:534:LEU:C	2.18	0.68
1:A:361:GLU:HG3	1:A:370:VAL:O	1.93	0.68
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.76	0.68
1:B:187:MET:HE3	1:B:296:TYR:CD1	2.29	0.68
1:B:200:ARG:NH2	2:B:749:HOH:O	2.27	0.67
1:B:547:LEU:HA	2:B:996:HOH:O	1.94	0.66
1:A:547:LEU:N	1:A:547:LEU:HD23	2.11	0.66
1:A:284:VAL:CG2	1:A:287:THR:HG22	2.26	0.66
1:A:508:ARG:CZ	1:A:530:VAL:HG11	2.25	0.66
1:A:538:PRO:HB2	2:A:792:HOH:O	1.95	0.66
1:B:200:ARG:HH11	1:B:204:LEU:HD11	1.61	0.66
1:A:398:GLU:HG2	1:A:403:THR:HG21	1.77	0.66
1:A:90:LYS:HG2	2:A:891:HOH:O	1.96	0.66
1:B:277:ARG:HH11	1:B:277:ARG:CG	2.07	0.66
1:A:1:SER:O	1:A:56:ARG:NH1	2.29	0.65
1:A:284:VAL:HG23	1:A:287:THR:HG22	1.79	0.65
1:B:303:CYS:SG	1:B:313:MET:CE	2.85	0.65
1:B:150:GLU:H	1:B:150:GLU:CD	2.03	0.64
1:A:539:ILE:HG23	1:A:540:PRO:HD2	1.80	0.63
1:A:461:GLN:HG3	1:A:542:ALA:HB2	1.79	0.63
1:A:74:LYS:O	1:A:77:THR:HB	1.97	0.63
1:A:148:GLN:NE2	1:A:150:GLU:HG2	2.12	0.63
1:B:109:ARG:NH1	1:B:109:ARG:CB	2.53	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:PRO:HG3	2:A:740:HOH:O	1.97	0.63
1:A:401:ARG:HG3	2:A:884:HOH:O	1.97	0.63
1:B:46:SER:HA	1:B:49:GLN:HE21	1.62	0.63
1:A:306:ALA:HB3	1:A:308:LEU:HD13	1.80	0.62
1:A:379:LYS:C	2:A:776:HOH:O	2.43	0.62
1:B:361:GLU:HG3	1:B:370:VAL:O	2.00	0.62
1:A:85:ILE:N	1:A:173:MET:HE3	2.15	0.62
1:B:359:ASP:HB3	1:B:362:LEU:HD22	1.80	0.62
1:A:439:LEU:N	1:A:439:LEU:HD22	2.15	0.61
1:A:520:THR:HA	1:A:523:ARG:HD2	1.82	0.61
1:A:512:LEU:C	1:A:514:GLN:H	2.08	0.61
1:B:158:ARG:HH11	1:B:158:ARG:CB	2.13	0.61
1:B:132:THR:O	1:B:259:ARG:HD3	2.00	0.61
1:A:28:ASN:OD1	1:A:34:HIS:CE1	2.54	0.61
1:B:547:LEU:H	1:B:547:LEU:CD1	2.14	0.61
1:A:237:GLU:OE2	1:A:254:ARG:HD2	2.01	0.61
1:A:346:TYR:O	1:A:347:SER:HB3	1.99	0.60
1:A:539:ILE:CG2	1:A:540:PRO:HD2	2.31	0.60
1:A:524:TYR:CD2	1:A:536:LEU:HD22	2.36	0.60
1:B:57:LEU:HD13	2:B:717:HOH:O	2.00	0.60
1:B:505:ARG:HH21	1:B:531:ARG:NE	1.99	0.60
1:A:148:GLN:CG	1:A:150:GLU:HG2	2.31	0.60
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.42	0.60
1:B:331:GLU:CD	1:B:331:GLU:H	2.07	0.60
1:A:365:SER:O	1:A:366:CYS:HB2	2.01	0.60
1:A:198:LYS:O	1:A:201:VAL:CG1	2.50	0.59
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.32	0.59
1:B:263:GLY:C	1:B:277:ARG:HH12	2.09	0.59
1:B:547:LEU:CD1	1:B:547:LEU:N	2.65	0.59
1:B:48:ARG:CZ	1:B:51:LYS:NZ	2.66	0.59
1:B:490:ARG:HA	1:B:490:ARG:NE	2.17	0.59
1:A:30:LEU:O	1:A:494:VAL:HG22	2.03	0.58
1:A:179:VAL:HG13	2:A:591:HOH:O	2.03	0.58
1:A:33:HIS:CE1	1:B:212:LYS:HE2	2.39	0.58
1:A:377:SER:HB3	2:A:771:HOH:O	2.03	0.58
1:A:405:ILE:CD1	1:A:446:GLN:HG2	2.29	0.58
1:A:24:ASN:O	2:A:774:HOH:O	2.17	0.58
1:B:464:GLU:HG3	1:B:469:LEU:CD1	2.32	0.58
1:A:268:ASN:HD21	1:A:272:GLN:NE2	2.02	0.58
1:B:277:ARG:NH2	2:B:628:HOH:O	2.31	0.57
1:A:540:PRO:HG2	1:A:541:ALA:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:HZ2	1:B:158:ARG:HH12	1.50	0.57
1:A:511:LEU:O	1:A:514:GLN:HB2	2.05	0.57
1:B:82:LEU:HD12	1:B:82:LEU:O	2.03	0.57
1:B:248:GLU:HG3	2:B:577:HOH:O	2.04	0.57
1:A:24:ASN:HB2	1:A:400:ALA:HB2	1.86	0.57
1:B:10:LEU:H	1:B:10:LEU:HD22	1.68	0.57
1:B:46:SER:HA	1:B:49:GLN:NE2	2.19	0.57
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.87	0.57
1:A:405:ILE:HD11	1:A:446:GLN:CG	2.29	0.56
1:A:24:ASN:HB2	1:A:400:ALA:CB	2.34	0.56
1:A:116:VAL:O	1:A:120:ARG:HG3	2.05	0.56
1:A:34:HIS:CD2	2:A:800:HOH:O	2.58	0.56
1:B:150:GLU:HA	2:B:914:HOH:O	2.06	0.56
1:B:503:ARG:O	1:B:507:VAL:HG23	2.06	0.56
1:B:200:ARG:HD3	1:B:384:LEU:HD11	1.88	0.56
1:B:263:GLY:HA2	1:B:277:ARG:NH1	2.21	0.56
1:A:187:MET:HE3	1:A:296:TYR:CD1	2.42	0.55
1:B:465:ARG:HE	1:B:546:ASP:CB	2.19	0.55
1:A:24:ASN:OD1	1:A:25:PRO:HD2	2.07	0.55
1:B:86:GLU:HG3	1:B:111:LEU:HD11	1.89	0.55
1:B:56:ARG:NH2	1:B:228:VAL:O	2.40	0.54
1:A:454:ILE:HA	1:A:566:ARG:O	2.07	0.54
1:A:461:GLN:N	1:A:461:GLN:OE1	2.39	0.54
1:B:457:LEU:HD13	1:B:517:ARG:HH11	1.72	0.54
1:B:327:ALA:C	1:B:331:GLU:HG3	2.33	0.54
1:A:212:LYS:HB2	1:A:212:LYS:NZ	2.22	0.54
1:A:364:THR:HG22	2:A:785:HOH:O	2.07	0.54
1:B:541:ALA:O	1:B:542:ALA:O	2.25	0.54
1:A:548:SER:OG	1:A:549:GLY:N	2.40	0.54
1:A:280:ARG:CD	1:A:291:ASN:OD1	2.55	0.54
1:B:465:ARG:HH21	1:B:546:ASP:CB	2.21	0.54
1:A:28:ASN:CB	2:A:774:HOH:O	2.53	0.53
1:B:547:LEU:H	1:B:547:LEU:HD13	1.72	0.53
1:B:556:SER:C	1:B:558:GLY:H	2.16	0.53
1:B:548:SER:O	1:B:549:GLY:C	2.51	0.53
1:B:491:LYS:HE3	2:B:663:HOH:O	2.08	0.53
1:B:280:ARG:HD2	1:B:291:ASN:OD1	2.09	0.53
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.91	0.53
1:A:374:HIS:HA	2:A:776:HOH:O	2.08	0.53
1:A:461:GLN:HB3	1:A:542:ALA:HA	1.91	0.53
1:B:457:LEU:CD1	1:B:517:ARG:NH1	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:HD22	1:A:356:PRO:HD3	1.91	0.53
1:A:24:ASN:ND2	1:A:27:SER:HB2	2.16	0.52
1:B:405:ILE:HD11	1:B:446:GLN:HG2	1.91	0.52
1:A:33:HIS:HE1	2:A:689:HOH:O	1.91	0.51
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.40	0.51
1:B:446:GLN:C	1:B:447:ILE:HD12	2.36	0.51
1:A:154:ARG:HG3	1:A:154:ARG:NH1	2.24	0.51
1:A:94:PRO:HA	1:A:109:ARG:HD2	1.93	0.51
1:A:510:LYS:HE2	2:A:787:HOH:O	2.10	0.51
1:A:24:ASN:HD22	1:A:27:SER:CA	2.23	0.51
1:A:531:ARG:NH2	2:A:865:HOH:O	2.43	0.51
1:A:375:ASP:O	1:A:376:ALA:C	2.53	0.51
1:A:379:LYS:O	1:A:380:ARG:C	2.53	0.51
1:B:130:THR:CB	2:B:800:HOH:O	2.13	0.51
1:B:337:ARG:CG	2:B:977:HOH:O	2.43	0.51
1:B:74:LYS:O	1:B:77:THR:HB	2.08	0.51
1:A:34:HIS:HD2	2:A:800:HOH:O	1.94	0.51
1:B:464:GLU:OE1	1:B:469:LEU:HD11	2.11	0.51
1:A:149:PRO:HB2	1:A:150:GLU:OE2	2.11	0.50
1:B:24:ASN:ND2	1:B:26:LEU:H	2.09	0.50
1:B:453:SER:HB2	1:B:563:SER:CB	2.42	0.50
1:A:403:THR:OG1	1:A:404:PRO:HD2	2.11	0.50
1:A:547:LEU:HG	1:A:565:SER:HA	1.94	0.50
1:A:284:VAL:O	1:A:287:THR:HG23	2.11	0.50
1:B:82:LEU:HD12	1:B:82:LEU:C	2.36	0.50
1:A:375:ASP:N	2:A:776:HOH:O	2.17	0.50
1:B:464:GLU:CD	1:B:469:LEU:HD11	2.36	0.50
1:A:4:TYR:CE1	1:A:52:VAL:HG13	2.46	0.50
1:B:562:HIS:CD2	2:B:821:HOH:O	2.65	0.50
1:A:439:LEU:H	1:A:439:LEU:CD2	2.25	0.49
1:B:93:PRO:HG2	1:B:96:SER:OG	2.12	0.49
1:B:453:SER:H	1:B:563:SER:HA	1.77	0.49
1:B:547:LEU:N	1:B:547:LEU:HD12	2.25	0.49
1:A:132:THR:O	1:A:259:ARG:HD3	2.12	0.49
1:A:505:ARG:NH2	1:A:531:ARG:HE	2.10	0.49
1:A:28:ASN:N	2:A:774:HOH:O	2.46	0.49
1:A:160:ILE:HD12	1:A:282:SER:OG	2.12	0.49
1:A:28:ASN:OD1	1:A:34:HIS:HE1	1.96	0.49
1:B:10:LEU:HD22	1:B:10:LEU:N	2.27	0.49
1:A:31:LEU:O	1:A:31:LEU:HD23	2.12	0.49
1:A:519:ALA:O	1:A:523:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HB2	1:A:173:MET:HA	1.94	0.49
1:B:79:LYS:HG3	1:B:244:ASP:HB3	1.93	0.49
1:A:508:ARG:NH2	1:A:530:VAL:HG11	2.28	0.48
1:B:346:TYR:O	1:B:347:SER:HB3	2.13	0.48
1:B:254:ARG:NH2	1:B:258:GLU:CG	2.76	0.48
1:A:26:LEU:HD11	1:A:432:ILE:HD12	1.95	0.48
1:B:153:GLY:HA2	2:B:982:HOH:O	2.12	0.48
1:B:337:ARG:HA	1:B:337:ARG:HE	1.78	0.48
1:A:542:ALA:C	1:A:544:GLN:H	2.20	0.48
1:A:56:ARG:HH11	1:A:56:ARG:CB	2.21	0.48
1:A:439:LEU:N	1:A:439:LEU:CD2	2.76	0.48
1:A:398:GLU:HG2	1:A:403:THR:CG2	2.44	0.48
1:A:31:LEU:HD23	1:A:31:LEU:C	2.38	0.48
1:B:48:ARG:CZ	1:B:51:LYS:HZ1	2.26	0.48
1:B:150:GLU:O	1:B:151:LYS:C	2.57	0.48
1:B:222:ARG:HG3	1:B:351:GLY:CA	2.42	0.47
1:B:109:ARG:NE	2:B:915:HOH:O	2.42	0.47
1:B:34:HIS:HD2	2:B:794:HOH:O	1.95	0.47
1:B:4:TYR:CE1	1:B:52:VAL:HG13	2.50	0.47
1:B:461:GLN:HB3	1:B:542:ALA:CA	2.32	0.47
1:B:505:ARG:NH1	2:B:613:HOH:O	2.47	0.47
1:A:284:VAL:HG22	1:A:287:THR:HG22	1.96	0.47
1:B:277:ARG:NH1	1:B:277:ARG:CG	2.74	0.47
1:B:237:GLU:OE2	1:B:254:ARG:HD2	2.14	0.47
1:A:328:GLY:HA3	1:A:331:GLU:HG2	1.97	0.47
1:B:200:ARG:NH1	2:B:635:HOH:O	2.47	0.47
1:A:220:ASP:HB3	2:A:867:HOH:O	2.16	0.46
1:B:434:LEU:HD11	1:B:514:GLN:NE2	2.30	0.46
1:B:457:LEU:HD12	1:B:517:ARG:NH1	2.31	0.46
1:B:523:ARG:HD3	1:B:534:LEU:HD21	1.97	0.46
1:B:284:VAL:HG23	1:B:287:THR:HG22	1.98	0.46
1:A:439:LEU:HD22	1:A:439:LEU:H	1.80	0.46
1:B:512:LEU:O	1:B:513:SER:C	2.57	0.46
1:A:457:LEU:HB3	1:A:517:ARG:HB3	1.98	0.46
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.98	0.46
1:B:453:SER:C	1:B:454:ILE:HG12	2.39	0.46
1:A:84:SER:C	1:A:173:MET:HE3	2.40	0.46
1:A:198:LYS:HB2	2:A:672:HOH:O	2.15	0.46
1:B:280:ARG:CD	1:B:291:ASN:OD1	2.63	0.46
1:A:227:THR:HB	1:A:347:SER:O	2.17	0.45
1:B:284:VAL:CG2	1:B:287:THR:HG22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:NH2	1:B:279:CYS:HB3	2.31	0.45
1:B:516:GLY:O	1:B:517:ARG:C	2.58	0.45
1:B:439:LEU:O	1:B:456:PRO:HG2	2.16	0.45
1:B:130:THR:CG2	2:B:680:HOH:O	2.60	0.45
1:A:85:ILE:HG13	1:A:173:MET:HE1	1.99	0.45
1:A:503:ARG:HG2	1:A:503:ARG:HH11	1.82	0.45
1:A:533:LYS:HD3	2:A:763:HOH:O	2.15	0.45
1:B:114:ARG:HG2	2:B:830:HOH:O	2.17	0.45
1:B:144:VAL:HG22	1:B:394:ARG:HG2	1.98	0.45
1:A:524:TYR:CG	1:A:536:LEU:HD22	2.51	0.45
1:B:24:ASN:ND2	1:B:26:LEU:N	2.64	0.45
1:B:106:LYS:HB2	1:B:106:LYS:NZ	2.32	0.45
1:A:85:ILE:HA	1:A:173:MET:HE3	1.98	0.45
1:A:464:GLU:HG3	1:A:469:LEU:CD1	2.47	0.45
1:A:503:ARG:CZ	2:A:906:HOH:O	2.65	0.45
1:B:365:SER:O	1:B:366:CYS:HB2	2.16	0.45
1:B:277:ARG:HE	1:B:281:ALA:HB2	1.82	0.45
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.85	0.44
1:A:428:HIS:O	1:A:432:ILE:HG12	2.17	0.44
1:A:440:GLU:O	1:A:441:LYS:C	2.60	0.44
1:B:517:ARG:NH1	1:B:517:ARG:HG3	2.32	0.44
1:A:512:LEU:C	1:A:514:GLN:N	2.74	0.44
1:B:1:SER:HA	2:B:908:HOH:O	2.17	0.44
1:B:490:ARG:NE	1:B:490:ARG:CA	2.79	0.44
1:A:24:ASN:CB	1:A:400:ALA:HB2	2.46	0.44
1:A:46:SER:HA	1:A:49:GLN:HE21	1.81	0.44
1:A:198:LYS:C	1:A:201:VAL:HG12	2.43	0.44
1:B:458:ASP:OD1	2:B:974:HOH:O	2.21	0.44
1:B:236:GLU:OE2	2:B:600:HOH:O	2.20	0.44
1:B:541:ALA:O	1:B:542:ALA:C	2.60	0.44
1:B:549:GLY:C	2:B:850:HOH:O	2.60	0.44
1:A:367:SER:O	1:A:386:ARG:HB2	2.18	0.44
1:A:512:LEU:HD23	1:A:512:LEU:HA	1.81	0.44
1:B:48:ARG:CZ	1:B:51:LYS:HZ3	2.31	0.44
1:B:96:SER:OG	1:B:559:ASP:OD1	2.36	0.44
1:A:32:ARG:HD2	2:A:825:HOH:O	2.17	0.44
1:A:514:GLN:HE21	1:A:514:GLN:HB3	1.56	0.44
1:B:82:LEU:C	1:B:82:LEU:CD1	2.91	0.44
1:B:556:SER:C	1:B:558:GLY:N	2.74	0.44
1:B:394:ARG:O	1:B:398:GLU:HG3	2.18	0.44
1:A:26:LEU:HD21	1:A:432:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:OE2	1:A:408:TRP:HD1	2.01	0.43
1:B:187:MET:HE3	1:B:296:TYR:CG	2.53	0.43
1:B:328:GLY:O	1:B:331:GLU:HG2	2.18	0.43
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.99	0.43
1:B:314:LEU:HD12	1:B:314:LEU:HA	1.84	0.43
1:B:448:TYR:HB2	2:B:747:HOH:O	2.19	0.43
1:A:201:VAL:HG13	1:A:202:GLU:N	2.33	0.43
1:A:154:ARG:HH11	1:A:154:ARG:CG	2.27	0.43
1:B:24:ASN:HD22	1:B:27:SER:H	1.67	0.43
1:B:5:THR:HG22	2:B:851:HOH:O	2.18	0.43
1:B:530:VAL:HG11	2:B:742:HOH:O	2.19	0.43
1:B:457:LEU:HD12	1:B:517:ARG:HH12	1.83	0.42
1:A:472:PHE:HE2	1:A:525:LEU:HD23	1.83	0.42
1:B:336:LEU:HD12	1:B:336:LEU:HA	1.83	0.42
1:A:308:LEU:N	1:A:308:LEU:HD12	2.34	0.42
1:A:430:PHE:O	1:A:434:LEU:HB2	2.19	0.42
1:A:524:TYR:CE2	1:A:536:LEU:HB3	2.55	0.42
1:B:447:ILE:HD12	1:B:447:ILE:N	2.34	0.42
1:B:148:GLN:O	1:B:149:PRO:C	2.62	0.42
1:B:434:LEU:CD1	1:B:514:GLN:NE2	2.82	0.42
1:A:306:ALA:HB3	1:A:308:LEU:CD1	2.47	0.42
1:A:148:GLN:HG2	1:A:150:GLU:HG2	2.01	0.42
1:A:150:GLU:O	1:A:151:LYS:C	2.62	0.42
1:B:83:LEU:HB2	1:B:173:MET:HA	2.00	0.42
1:A:85:ILE:CA	1:A:173:MET:HE3	2.50	0.42
1:A:148:GLN:HG2	1:A:150:GLU:N	2.25	0.42
1:A:416:ALA:N	1:A:417:PRO:HD3	2.35	0.42
1:A:483:ASN:HD22	1:A:483:ASN:HA	1.65	0.41
1:A:306:ALA:CB	1:A:308:LEU:CD1	2.97	0.41
1:A:499:THR:HG23	2:B:723:HOH:O	2.20	0.41
1:B:153:GLY:CA	2:B:982:HOH:O	2.68	0.41
1:B:531:ARG:NH2	2:B:890:HOH:O	2.32	0.41
1:A:20:LYS:O	1:A:22:PRO:CD	2.53	0.41
1:B:92:THR:HA	1:B:93:PRO:HD2	1.73	0.41
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.87	0.41
1:B:457:LEU:HD13	1:B:517:ARG:NH1	2.34	0.41
1:A:148:GLN:HG3	1:A:149:PRO:HD2	2.01	0.41
1:A:464:GLU:OE2	1:A:538:PRO:HA	2.21	0.41
1:B:106:LYS:HB3	2:B:932:HOH:O	2.20	0.41
1:A:416:ALA:N	1:A:417:PRO:CD	2.83	0.41
1:B:86:GLU:OE2	1:B:90:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:HD3	2:B:883:HOH:O	2.20	0.41
1:A:22:PRO:CD	2:A:653:HOH:O	2.69	0.41
1:A:26:LEU:CD1	1:A:432:ILE:HD12	2.50	0.41
1:B:461:GLN:OE1	1:B:461:GLN:N	2.40	0.41
1:A:219:TYR:HE2	1:A:221:THR:HG22	1.85	0.41
1:A:346:TYR:O	1:A:347:SER:CB	2.67	0.41
1:B:150:GLU:CA	2:B:914:HOH:O	2.68	0.41
1:A:93:PRO:HB3	1:A:561:TYR:HB2	2.03	0.41
1:A:150:GLU:N	1:A:150:GLU:CD	2.79	0.41
1:A:508:ARG:CZ	1:A:530:VAL:CG1	2.97	0.41
1:B:84:SER:OG	1:B:87:GLU:HG3	2.21	0.40
1:B:104:GLY:O	1:B:107:ASP:HB2	2.20	0.40
1:B:187:MET:HE3	1:B:296:TYR:HB2	2.02	0.40
1:A:308:LEU:N	1:A:308:LEU:CD1	2.83	0.40
1:A:27:SER:HB3	2:A:650:HOH:O	2.20	0.40
1:A:309:GLN:O	1:A:324:CYS:HB2	2.21	0.40
1:A:331:GLU:OE1	1:A:331:GLU:N	2.55	0.40
1:A:541:ALA:O	1:A:542:ALA:C	2.64	0.40
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.51	0.40
1:B:508:ARG:NE	2:B:742:HOH:O	2.29	0.40
1:A:366:CYS:O	1:A:367:SER:HB2	2.21	0.40
1:A:544:GLN:O	1:A:546:ASP:N	2.52	0.40
1:B:44:SER:O	1:B:47:LEU:HB2	2.21	0.40
1:B:517:ARG:HH11	1:B:517:ARG:CG	2.34	0.40
1:B:555:TYR:O	1:B:556:SER:C	2.65	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	564/570 (99%)	532 (94%)	23 (4%)	9 (2%)	7 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	563/570 (99%)	529 (94%)	22 (4%)	12 (2%)	5	2
All	All	1127/1140 (99%)	1061 (94%)	45 (4%)	21 (2%)	6	3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	A	540	PRO
1	A	542	ALA
1	A	545	LEU
1	B	103	TYR
1	B	540	PRO
1	B	542	ALA
1	B	548	SER
1	B	549	GLY
1	B	556	SER
1	A	23	ILE
1	A	543	SER
1	B	515	GLY
1	B	563	SER
1	B	149	PRO
1	A	380	ARG
1	B	547	LEU
1	A	26	LEU
1	B	151	LYS
1	B	544	GLN
1	A	376	ALA

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	475/485 (98%)	439 (92%)	36 (8%)	12	9
1	B	475/485 (98%)	422 (89%)	53 (11%)	6	3
All	All	950/970 (98%)	861 (91%)	89 (9%)	8	5

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	26	LEU
1	A	28	ASN
1	A	31	LEU
1	A	47	LEU
1	A	52	VAL
1	A	56	ARG
1	A	68	LEU
1	A	77	THR
1	A	106	LYS
1	A	126	LEU
1	A	130	THR
1	A	144	VAL
1	A	150	GLU
1	A	179	VAL
1	A	210	SER
1	A	212	LYS
1	A	287	THR
1	A	313	MET
1	A	316	ASN
1	A	322	VAL
1	A	330	GLN
1	A	331	GLU
1	A	345	ARG
1	A	362	LEU
1	A	384	LEU
1	A	386	ARG
1	A	412	ILE
1	A	425	LEU
1	A	433	LEU
1	A	434	LEU
1	A	439	LEU
1	A	459	LEU
1	A	514	GLN
1	A	534	LEU
1	A	547	LEU
1	B	10	LEU
1	B	20	LYS
1	B	24	ASN
1	B	47	LEU
1	B	52	VAL
1	B	56	ARG

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Mol	Chain	Res	Type
1	B	57	LEU
1	B	68	LEU
1	B	77	THR
1	B	82	LEU
1	B	94	PRO
1	B	96	SER
1	B	106	LYS
1	B	109	ARG
1	B	116	VAL
1	B	126	LEU
1	B	130	THR
1	B	144	VAL
1	B	148	GLN
1	B	149	PRO
1	B	150	GLU
1	B	158	ARG
1	B	163	PRO
1	B	180	SER
1	B	197	PRO
1	B	221	THR
1	B	222	ARG
1	B	259	ARG
1	B	262	ILE
1	B	274	CYS
1	B	277	ARG
1	B	287	THR
1	B	308	LEU
1	B	310	ASP
1	B	313	MET
1	B	330	GLN
1	B	331	GLU
1	B	337	ARG
1	B	362	LEU
1	B	364	THR
1	B	367	SER
1	B	405	ILE
1	B	425	LEU
1	B	439	LEU
1	B	453	SER
1	B	454	ILE
1	B	459	LEU
1	B	490	ARG

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Mol	Chain	Res	Type
1	B	517	ARG
1	B	531	ARG
1	B	534	LEU
1	B	538	PRO
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	33	HIS
1	A	34	HIS
1	A	35	ASN
1	A	49	GLN
1	A	110	ASN
1	A	184	GLN
1	A	206	ASN
1	A	272	GLN
1	A	309	GLN
1	A	316	ASN
1	A	428	HIS
1	A	436	GLN
1	A	446	GLN
1	A	483	ASN
1	A	514	GLN
1	B	24	ASN
1	B	28	ASN
1	B	34	HIS
1	B	35	ASN
1	B	49	GLN
1	B	148	GLN
1	B	206	ASN
1	B	273	ASN
1	B	374	HIS
1	B	483	ASN
1	B	514	GLN

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.