



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:49 AM UTC

PDB ID : 2W4B / pdb_00002w4b
Title : Epstein-Barr virus alkaline nuclease D203S mutant
Authors : Buisson, M.; Geoui, T.; Flot, D.; Tarbouriech, N.; Burmeister, W.P.
Deposited on : 2008-11-24
Resolution : 3.50 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

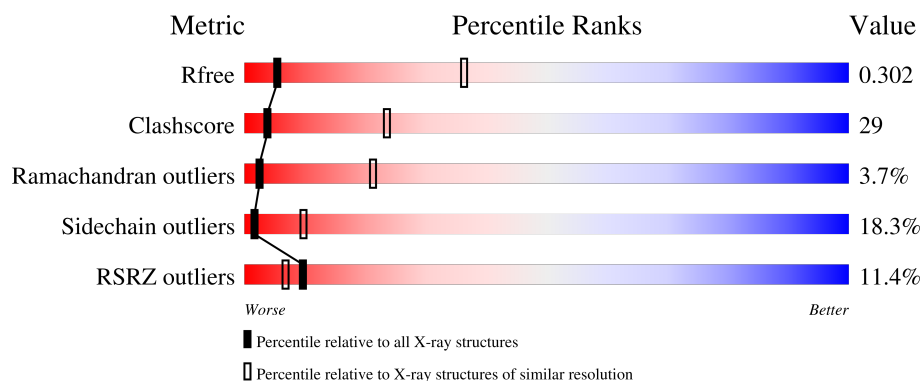
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	470	14% 49% 34% 11% • •
1	B	470	8% 46% 34% 10% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7041 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 ALKALINE EXONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	1
			3587	2288	605	672	22			
1	B	439	Total	C	N	O	S	0	0	1
			3454	2205	582	645	22			

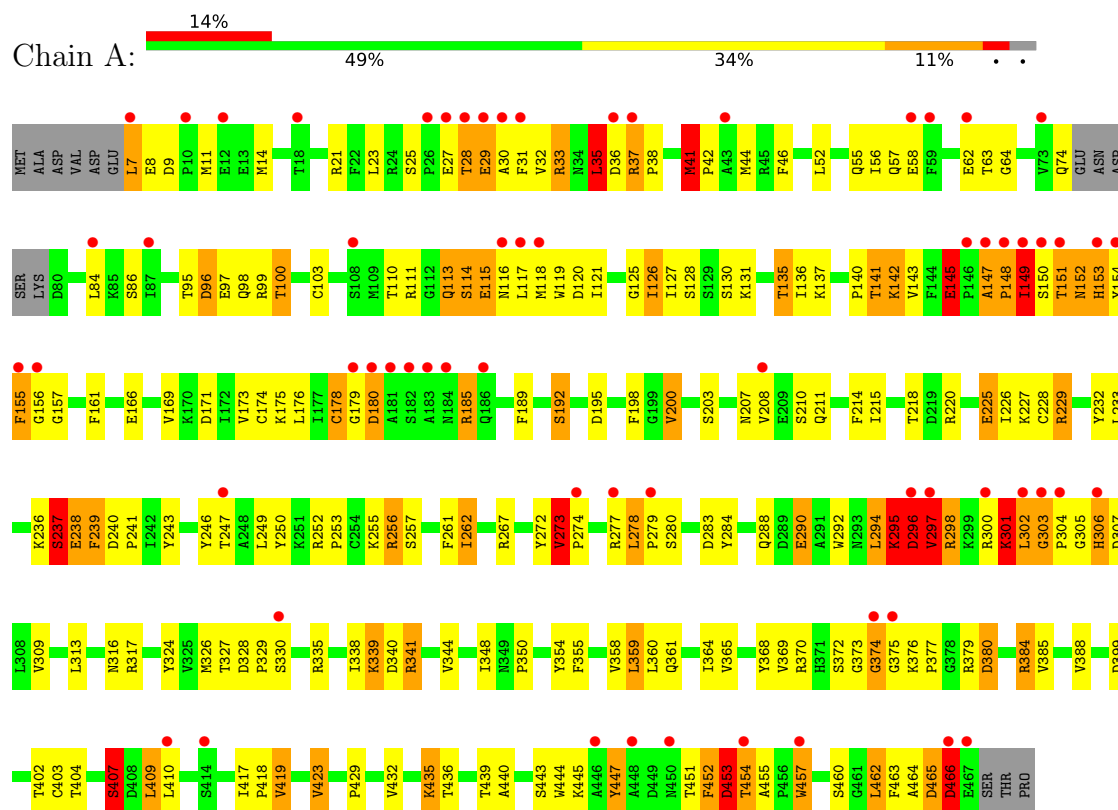
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	ASP	engineered mutation	UNP P03217
B	203	SER	ASP	engineered mutation	UNP P03217

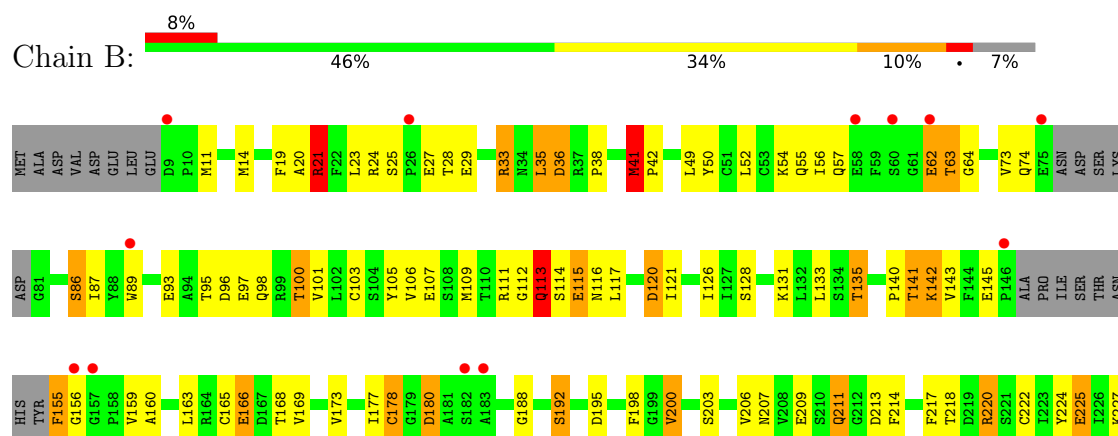
3 Residue-property plots

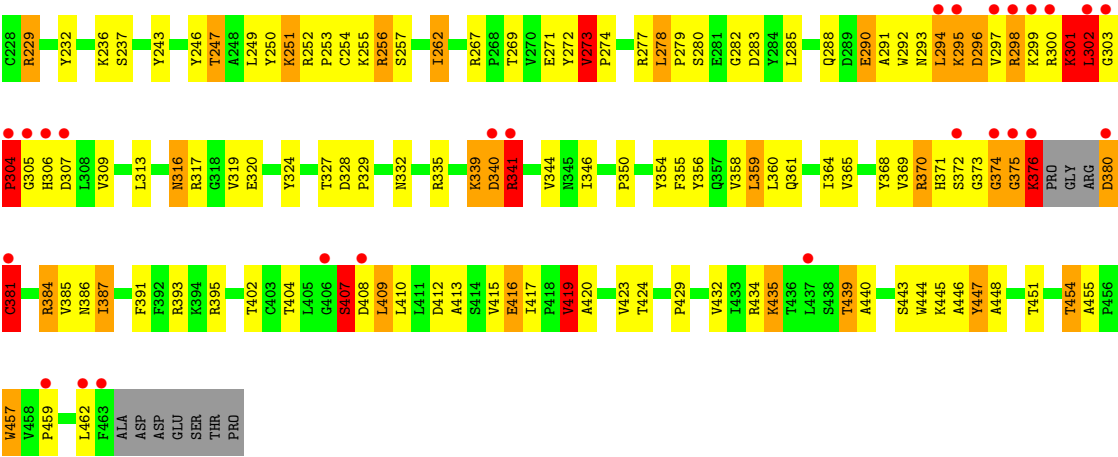
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: ALKALINE EXONUCLEASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.51Å 63.79Å 114.13Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	31.19 – 3.50 31.19 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.8 (31.19-3.50) 99.7 (31.19-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.190 , 0.256 0.262 , 0.302	Depositor DCC
R_{free} test set	1295 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7041	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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	1.65	8/3674 (0.2%)	1.47	34/4987 (0.7%)
1	B	1.27	9/3534 (0.3%)	1.39	38/4791 (0.8%)
All	All	1.48	17/7208 (0.2%)	1.43	72/9778 (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	8
1	B	0	4
All	All	0	12

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	PHE	C-N	-66.39	0.40	1.33
1	B	35	LEU	C-N	-39.41	0.85	1.33
1	A	453	ASP	C-N	-34.48	0.80	1.34
1	A	36	ASP	C-N	-13.70	1.13	1.33
1	B	36	ASP	C-N	-12.80	1.07	1.33
1	B	180	ASP	CA-C	-6.47	1.44	1.52
1	B	387	ILE	C-O	-6.44	1.17	1.24
1	B	178	CYS	CA-C	-6.01	1.50	1.53
1	A	301	LYS	CA-C	-5.95	1.45	1.53
1	A	273	VAL	CA-CB	5.79	1.58	1.54
1	B	304	PRO	C-N	5.68	1.41	1.33
1	A	297	VAL	CA-CB	-5.65	1.49	1.55
1	A	466	ASP	C-N	-5.51	1.25	1.33
1	B	376	LYS	CA-CB	5.41	1.64	1.53
1	B	21	ARG	C-O	-5.38	1.17	1.24
1	A	149	ILE	CA-CB	5.35	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	301	LYS	CA-C	-5.12	1.46	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LEU	CA-C-N	24.51	168.35	121.54
1	A	35	LEU	C-N-CA	24.51	168.35	121.54
1	A	452	PHE	O-C-N	-22.80	92.27	122.59
1	A	35	LEU	O-C-N	-19.22	100.86	123.16
1	A	452	PHE	CA-C-N	19.11	158.05	121.54
1	A	452	PHE	C-N-CA	19.11	158.05	121.54
1	B	36	ASP	O-C-N	-17.22	104.12	122.03
1	B	35	LEU	CA-C-N	16.92	142.98	120.65
1	B	35	LEU	C-N-CA	16.92	142.98	120.65
1	B	35	LEU	O-C-N	-13.25	107.37	123.01
1	B	301	LYS	N-CA-C	10.68	133.55	110.80
1	B	113	GLN	N-CA-C	10.20	125.67	112.41
1	B	304	PRO	CA-N-CD	-9.23	99.08	112.00
1	A	374	GLY	N-CA-C	8.81	131.14	115.80
1	B	302	LEU	N-CA-CB	8.70	125.19	110.49
1	A	192	SER	CA-C-N	7.97	127.54	118.85
1	A	192	SER	C-N-CA	7.97	127.54	118.85
1	A	451	THR	N-CA-C	-7.94	104.74	114.75
1	B	64	GLY	N-CA-C	7.68	121.94	112.64
1	A	147	ALA	CA-C-N	7.34	129.01	119.84
1	A	147	ALA	C-N-CA	7.34	129.01	119.84
1	A	239	PHE	CA-C-N	-7.10	110.52	120.39
1	A	239	PHE	C-N-CA	-7.10	110.52	120.39
1	B	156	GLY	N-CA-C	-7.07	96.42	113.18
1	A	64	GLY	N-CA-C	6.94	121.03	112.64
1	B	341	ARG	N-CA-C	6.66	117.93	108.54
1	B	381	CYS	N-CA-CB	-6.66	99.24	110.49
1	A	237	SER	N-CA-C	6.43	118.54	107.93
1	B	290	GLU	N-CA-C	6.27	118.12	111.28
1	A	297	VAL	N-CA-C	6.25	116.50	107.88
1	B	192	SER	CA-C-N	6.21	125.78	119.19
1	B	192	SER	C-N-CA	6.21	125.78	119.19
1	B	419	VAL	N-CA-C	-6.19	106.73	111.62
1	B	451	THR	N-CA-C	-6.01	106.93	114.56
1	A	403	CYS	N-CA-C	5.99	119.30	108.69
1	B	63	THR	CA-C-N	5.97	126.74	119.99
1	B	63	THR	C-N-CA	5.97	126.74	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	ASP	O-C-N	-5.95	114.67	122.59
1	A	185	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	A	145	GLU	N-CA-C	5.74	118.81	110.14
1	B	419	VAL	CB-CA-C	5.69	116.11	111.05
1	B	273	VAL	CA-C-N	5.64	125.40	119.76
1	B	273	VAL	C-N-CA	5.64	125.40	119.76
1	B	375	GLY	N-CA-C	-5.63	103.95	112.84
1	B	165	CYS	N-CA-C	5.59	120.23	113.41
1	B	341	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	B	316	ASN	N-CA-C	5.56	120.22	113.38
1	A	97	GLU	CB-CA-C	-5.56	101.92	110.81
1	A	226	ILE	N-CA-C	5.53	116.27	108.36
1	B	416	GLU	CA-C-N	-5.53	118.61	122.59
1	B	416	GLU	C-N-CA	-5.53	118.61	122.59
1	B	340	ASP	N-CA-C	5.52	117.66	108.99
1	A	114	SER	N-CA-C	-5.51	106.51	113.18
1	A	295	LYS	N-CA-C	5.38	122.27	110.80
1	B	376	LYS	CG-CD-CE	-5.35	99.00	111.30
1	B	41	MET	N-CA-C	5.33	118.32	108.94
1	B	211	GLN	N-CA-C	-5.29	99.24	109.24
1	B	293	ASN	N-CA-C	5.28	117.69	108.76
1	A	41	MET	N-CA-C	5.24	118.17	108.94
1	B	178	CYS	CA-C-O	5.23	121.63	118.33
1	A	114	SER	CA-C-N	5.22	129.55	120.68
1	A	114	SER	C-N-CA	5.22	129.55	120.68
1	B	120	ASP	N-CA-C	5.17	116.60	111.07
1	A	185	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A	180	ASP	N-CA-C	5.05	117.63	108.69
1	A	290	GLU	N-CA-C	5.05	116.78	111.28
1	A	125	GLY	N-CA-C	-5.04	108.16	115.27
1	B	62	GLU	CA-CB-CG	5.01	124.13	114.10
1	A	273	VAL	CB-CA-C	5.01	115.22	110.16
1	A	96	ASP	N-CA-C	5.01	117.39	111.33
1	B	387	ILE	CA-C-N	5.00	128.56	121.66
1	B	387	ILE	C-N-CA	5.00	128.56	121.66

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	ILE	Peptide
1	A	150	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	35	LEU	Peptide
1	A	407	SER	Peptide
1	A	41	MET	Peptide
1	A	452	PHE	Peptide,Mainchain
1	A	453	ASP	Mainchain
1	B	112	GLY	Peptide
1	B	380	ASP	Peptide
1	B	407	SER	Peptide
1	B	41	MET	Peptide

5.2 Too-close contacts [i](#)

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	3587	0	3538	212	5
1	B	3454	0	3417	197	1
All	All	7041	0	6955	401	5

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 29.

All (401) 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:453:ASP:C	1:A:454:THR:CA	2.00	1.35
1:B:271:GLU:OE1	1:B:298:ARG:NH1	1.60	1.32
1:A:116:ASN:OD1	1:A:117:LEU:N	1.65	1.28
1:B:302:LEU:O	1:B:304:PRO:HD3	1.34	1.26
1:A:95:THR:HG21	1:B:178:CYS:O	1.38	1.23
1:B:35:LEU:O	1:B:36:ASP:N	1.68	1.21
1:A:453:ASP:O	1:A:454:THR:N	1.72	1.20
1:A:453:ASP:CA	1:A:454:THR:N	2.04	1.20
1:A:335:ARG:NH1	1:A:407:SER:HA	1.57	1.19
1:A:208:VAL:HG11	1:A:215:ILE:CG2	1.77	1.15
1:B:35:LEU:C	1:B:36:ASP:CA	2.19	1.15
1:A:300:ARG:HE	1:A:302:LEU:HG	1.03	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLN:O	1:B:115:GLU:N	1.81	1.12
1:B:256:ARG:HG2	1:B:256:ARG:HH11	1.04	1.12
1:A:384:ARG:HH11	1:A:384:ARG:HG2	1.03	1.09
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.18	1.08
1:B:387:ILE:O	1:B:387:ILE:HD12	1.49	1.08
1:B:384:ARG:HG2	1:B:384:ARG:HH11	1.09	1.07
1:B:375:GLY:O	1:B:376:LYS:HE2	1.56	1.05
1:B:387:ILE:HD11	1:B:424:THR:OG1	1.56	1.05
1:B:35:LEU:CA	1:B:36:ASP:N	2.18	1.04
1:A:301:LYS:HE2	1:A:301:LYS:O	1.60	1.00
1:A:208:VAL:CG1	1:A:215:ILE:CG2	2.40	0.99
1:B:277:ARG:HD2	1:B:298:ARG:O	1.63	0.98
1:A:236:LYS:HD2	1:A:243:TYR:HE1	1.26	0.98
1:B:142:LYS:H	1:B:142:LYS:HD2	1.25	0.97
1:B:302:LEU:C	1:B:304:PRO:HD3	1.89	0.96
1:B:35:LEU:C	1:B:36:ASP:N	0.85	0.95
1:B:301:LYS:HG2	1:B:302:LEU:N	1.80	0.94
1:A:335:ARG:HH12	1:A:407:SER:HA	1.14	0.93
1:A:141:THR:HG23	1:A:447:TYR:HE1	1.30	0.93
1:A:236:LYS:HD2	1:A:243:TYR:CE1	2.03	0.93
1:A:294:LEU:O	1:A:295:LYS:HB3	1.65	0.93
1:A:335:ARG:HH12	1:A:407:SER:CA	1.82	0.92
1:A:142:LYS:HD2	1:A:142:LYS:H	1.33	0.91
1:A:149:ILE:HG12	1:A:151:THR:HA	1.51	0.91
1:A:295:LYS:O	1:A:296:ASP:HB3	1.68	0.90
1:B:302:LEU:O	1:B:304:PRO:CD	2.19	0.90
1:A:453:ASP:C	1:A:454:THR:N	0.80	0.90
1:A:253:PRO:HG2	1:A:340:ASP:OD1	1.72	0.89
1:A:453:ASP:O	1:A:454:THR:CA	2.12	0.89
1:A:330:SER:OG	1:A:399:ASP:OD2	1.91	0.89
1:A:116:ASN:OD1	1:A:118:MET:N	2.05	0.88
1:A:57:GLN:HE21	1:A:63:THR:HG22	1.38	0.88
1:A:300:ARG:NE	1:A:302:LEU:HG	1.88	0.88
1:A:384:ARG:HG2	1:A:384:ARG:NH1	1.83	0.87
1:B:384:ARG:HH11	1:B:384:ARG:CG	1.88	0.86
1:A:152:ASN:OD1	1:A:155:PHE:HE2	1.59	0.86
1:A:301:LYS:O	1:A:302:LEU:HD23	1.76	0.86
1:B:335:ARG:NH1	1:B:407:SER:HA	1.90	0.85
1:B:141:THR:HG23	1:B:447:TYR:HE1	1.40	0.85
1:B:128:SER:HB3	1:B:131:LYS:HD2	1.59	0.84
1:B:236:LYS:HD2	1:B:243:TYR:CE1	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ARG:HG2	1:B:384:ARG:NH1	1.84	0.84
1:A:95:THR:CG2	1:B:178:CYS:O	2.23	0.84
1:A:208:VAL:HG11	1:A:215:ILE:HG23	1.58	0.83
1:B:21:ARG:NH2	1:B:25:SER:OG	2.12	0.83
1:A:7:LEU:N	1:A:7:LEU:HD22	1.94	0.83
1:B:327:THR:HG22	1:B:339:LYS:HB2	1.60	0.83
1:A:208:VAL:CG1	1:A:215:ILE:HG23	2.05	0.82
1:B:142:LYS:H	1:B:142:LYS:CD	1.90	0.82
1:B:225:GLU:HG3	1:B:227:LYS:HE2	1.60	0.82
1:B:236:LYS:HD2	1:B:243:TYR:HE1	1.46	0.81
1:A:128:SER:HB3	1:A:131:LYS:HD2	1.62	0.81
1:A:301:LYS:O	1:A:301:LYS:HG2	1.78	0.81
1:A:453:ASP:O	1:A:454:THR:HA	1.80	0.81
1:A:7:LEU:N	1:A:7:LEU:CD2	2.44	0.80
1:B:300:ARG:NH2	1:B:302:LEU:HD21	1.97	0.80
1:A:294:LEU:O	1:A:295:LYS:CB	2.29	0.80
1:A:301:LYS:O	1:A:302:LEU:CD2	2.30	0.80
1:A:300:ARG:HE	1:A:302:LEU:CG	1.91	0.79
1:B:365:VAL:O	1:B:369:VAL:HG23	1.81	0.79
1:B:370:ARG:HD2	1:B:371:HIS:CE1	2.18	0.79
1:A:295:LYS:O	1:A:296:ASP:CB	2.30	0.78
1:B:229:ARG:NH2	1:B:283:ASP:OD1	2.16	0.78
1:B:387:ILE:O	1:B:387:ILE:CD1	2.30	0.78
1:A:301:LYS:O	1:A:301:LYS:CE	2.32	0.78
1:A:341:ARG:HH11	1:A:341:ARG:HB2	1.49	0.78
1:B:256:ARG:HG2	1:B:256:ARG:NH1	1.84	0.78
1:B:387:ILE:HG13	1:B:424:THR:HB	1.66	0.78
1:B:131:LYS:O	1:B:135:THR:HB	1.84	0.77
1:A:113:GLN:OE1	1:A:116:ASN:CB	2.33	0.77
1:B:141:THR:HG23	1:B:447:TYR:CE1	2.20	0.77
1:B:250:TYR:HE2	1:B:339:LYS:HD3	1.49	0.77
1:A:211:GLN:HB2	1:A:214:PHE:HB2	1.66	0.77
1:A:141:THR:HG23	1:A:447:TYR:CE1	2.17	0.77
1:A:301:LYS:O	1:A:301:LYS:CG	2.30	0.76
1:B:173:VAL:HA	1:B:177:ILE:HD12	1.68	0.76
1:B:253:PRO:HG2	1:B:340:ASP:OD1	1.86	0.76
1:A:142:LYS:H	1:A:142:LYS:CD	1.99	0.76
1:A:296:ASP:CG	1:A:297:VAL:H	1.93	0.76
1:A:208:VAL:CG1	1:A:215:ILE:HG22	2.14	0.75
1:B:304:PRO:HD2	1:B:306:HIS:HB2	1.67	0.75
1:A:154:TYR:CG	1:A:154:TYR:O	2.40	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:O	1:A:155:PHE:C	2.30	0.75
1:A:116:ASN:OD1	1:A:116:ASN:C	2.30	0.74
1:A:174:CYS:O	1:A:178:CYS:O	2.05	0.73
1:B:271:GLU:CD	1:B:298:ARG:NH1	2.47	0.73
1:A:375:GLY:O	1:B:384:ARG:NH2	2.23	0.72
1:A:296:ASP:CG	1:A:297:VAL:N	2.44	0.72
1:A:151:THR:O	1:A:152:ASN:HB2	1.90	0.71
1:B:211:GLN:HB2	1:B:214:PHE:HB2	1.70	0.71
1:A:207:ASN:ND2	1:A:220:ARG:O	2.22	0.70
1:A:227:LYS:HE3	1:A:354:TYR:CD1	2.26	0.70
1:B:435:LYS:O	1:B:439:THR:HG23	1.92	0.70
1:A:256:ARG:HG2	1:A:256:ARG:NH1	1.95	0.70
1:B:404:THR:HA	1:B:409:LEU:O	1.92	0.69
1:A:237:SER:O	1:A:238:GLU:C	2.35	0.69
1:B:141:THR:O	1:B:145:GLU:HG2	1.92	0.69
1:B:376:LYS:HG2	1:B:380:ASP:CA	2.23	0.69
1:A:229:ARG:NH2	1:A:283:ASP:OD1	2.25	0.69
1:B:387:ILE:HD12	1:B:387:ILE:C	2.16	0.69
1:A:238:GLU:O	1:A:239:PHE:HB2	1.91	0.68
1:A:341:ARG:O	1:A:341:ARG:HG3	1.92	0.68
1:A:152:ASN:OD1	1:A:155:PHE:CE2	2.44	0.68
1:A:145:GLU:HA	1:A:145:GLU:OE1	1.92	0.68
1:A:250:TYR:HE2	1:A:339:LYS:HD3	1.57	0.68
1:B:89:TRP:HZ3	1:B:93:GLU:OE2	1.75	0.68
1:B:387:ILE:CG1	1:B:424:THR:HB	2.25	0.67
1:A:28:THR:HG22	1:A:29:GLU:N	2.07	0.67
1:B:227:LYS:HE3	1:B:354:TYR:CD1	2.31	0.66
1:B:372:SER:C	1:B:374:GLY:H	2.03	0.66
1:A:149:ILE:HD11	1:A:153:HIS:NE2	2.11	0.66
1:A:11:MET:HE1	1:A:121:ILE:HD12	1.78	0.66
1:A:208:VAL:HG11	1:A:215:ILE:HG21	1.76	0.65
1:A:249:LEU:HA	1:A:257:SER:OG	1.96	0.65
1:A:141:THR:O	1:A:145:GLU:HG2	1.97	0.65
1:A:278:LEU:HB2	1:A:301:LYS:HB2	1.79	0.64
1:B:145:GLU:OE1	1:B:145:GLU:HA	1.97	0.64
1:B:387:ILE:HD11	1:B:424:THR:CB	2.28	0.64
1:B:113:GLN:C	1:B:115:GLU:H	1.91	0.63
1:A:305:GLY:C	1:A:307:ASP:H	2.06	0.63
1:A:171:ASP:HA	1:A:185:ARG:HH12	1.62	0.62
1:B:169:VAL:O	1:B:173:VAL:HG23	1.99	0.62
1:B:335:ARG:HH12	1:B:407:SER:HA	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:HH11	1:A:384:ARG:CG	1.94	0.62
1:B:324:TYR:CE2	1:B:341:ARG:HD3	2.34	0.62
1:A:236:LYS:CD	1:A:243:TYR:HE1	2.07	0.62
1:A:301:LYS:C	1:A:302:LEU:HD23	2.25	0.62
1:B:14:MET:HE1	1:B:55:GLN:NE2	2.14	0.62
1:A:303:GLY:O	1:A:305:GLY:N	2.33	0.62
1:A:131:LYS:O	1:A:135:THR:HB	1.98	0.61
1:B:96:ASP:O	1:B:100:THR:HG23	2.00	0.61
1:A:290:GLU:C	1:A:292:TRP:H	2.08	0.61
1:A:96:ASP:O	1:A:100:THR:HG23	2.00	0.61
1:B:301:LYS:CG	1:B:302:LEU:N	2.58	0.61
1:A:466:ASP:OD1	1:B:256:ARG:NH1	2.33	0.61
1:B:391:PHE:CD1	1:B:420:ALA:HB3	2.36	0.61
1:A:335:ARG:HH11	1:A:407:SER:HA	1.61	0.60
1:B:391:PHE:HD1	1:B:420:ALA:HB3	1.65	0.60
1:A:327:THR:HG22	1:A:339:LYS:HB2	1.83	0.60
1:B:236:LYS:CD	1:B:243:TYR:HE1	2.12	0.60
1:B:372:SER:O	1:B:374:GLY:N	2.24	0.60
1:A:278:LEU:HD13	1:A:306:HIS:CD2	2.35	0.60
1:B:335:ARG:HH12	1:B:407:SER:HB3	1.66	0.60
1:B:141:THR:CG2	1:B:447:TYR:HE1	2.13	0.60
1:A:250:TYR:CE2	1:A:339:LYS:HD3	2.37	0.60
1:A:192:SER:HB3	1:A:195:ASP:OD2	2.02	0.60
1:B:359:LEU:C	1:B:359:LEU:HD23	2.27	0.60
1:A:113:GLN:OE1	1:A:116:ASN:HB3	2.01	0.59
1:A:225:GLU:OE1	1:A:225:GLU:HA	2.00	0.59
1:B:142:LYS:HD2	1:B:142:LYS:N	2.07	0.59
1:A:154:TYR:O	1:A:154:TYR:CD2	2.56	0.59
1:A:37:ARG:NH1	1:B:332:ASN:HD21	2.00	0.58
1:A:27:GLU:O	1:A:30:ALA:HB3	2.03	0.58
1:B:89:TRP:CZ3	1:B:93:GLU:OE2	2.57	0.58
1:A:365:VAL:O	1:A:369:VAL:HG23	2.02	0.58
1:A:113:GLN:OE1	1:A:116:ASN:HB2	2.03	0.58
1:A:303:GLY:O	1:A:307:ASP:OD2	2.21	0.58
1:B:198:PHE:HB3	1:B:360:LEU:HD21	1.84	0.58
1:B:247:THR:O	1:B:251:LYS:HG2	2.03	0.58
1:A:116:ASN:CG	1:A:117:LEU:N	2.53	0.58
1:B:454:THR:O	1:B:455:ALA:C	2.46	0.58
1:A:154:TYR:C	1:A:155:PHE:O	2.46	0.57
1:B:301:LYS:HG2	1:B:302:LEU:H	1.65	0.57
1:B:429:PRO:HB2	1:B:432:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:TYR:CE2	1:B:339:LYS:HD3	2.35	0.57
1:A:460:SER:HA	1:A:463:PHE:CD1	2.40	0.57
1:A:341:ARG:O	1:A:341:ARG:CG	2.48	0.57
1:B:52:LEU:HG	1:B:56:ILE:HD12	1.86	0.57
1:B:200:VAL:HG21	1:B:361:GLN:HA	1.85	0.57
1:B:375:GLY:O	1:B:376:LYS:CE	2.44	0.56
1:B:272:TYR:CE1	1:B:274:PRO:HG3	2.41	0.56
1:B:375:GLY:C	1:B:376:LYS:HE2	2.28	0.56
1:A:379:ARG:NH2	1:A:379:ARG:HG3	2.21	0.56
1:A:440:ALA:O	1:A:443:SER:HB3	2.06	0.56
1:A:278:LEU:HD13	1:A:306:HIS:NE2	2.20	0.56
1:B:11:MET:HE1	1:B:121:ILE:HD12	1.87	0.56
1:B:115:GLU:OE2	1:B:115:GLU:HA	2.06	0.56
1:B:376:LYS:HG2	1:B:380:ASP:HA	1.88	0.56
1:A:31:PHE:CD2	1:A:84:LEU:HB3	2.41	0.55
1:A:429:PRO:HB2	1:A:432:VAL:HG23	1.88	0.55
1:A:454:THR:O	1:A:455:ALA:C	2.49	0.55
1:A:198:PHE:HB3	1:A:360:LEU:HD21	1.88	0.55
1:B:103:CYS:HB3	1:B:368:TYR:OH	2.07	0.55
1:A:38:PRO:HB2	1:A:457:TRP:HD1	1.71	0.55
1:B:304:PRO:CD	1:B:306:HIS:HB2	2.34	0.55
1:A:33:ARG:HA	1:A:33:ARG:NE	2.21	0.54
1:A:388:VAL:HG22	1:A:423:VAL:HG13	1.89	0.54
1:A:141:THR:CG2	1:A:447:TYR:HE1	2.13	0.54
1:A:295:LYS:O	1:A:295:LYS:CG	2.53	0.54
1:A:435:LYS:O	1:A:436:THR:C	2.49	0.54
1:A:295:LYS:O	1:A:295:LYS:HG3	2.07	0.54
1:A:301:LYS:O	1:A:302:LEU:HD22	2.07	0.54
1:B:335:ARG:HH12	1:B:407:SER:CA	2.20	0.54
1:A:200:VAL:HG21	1:A:361:GLN:HA	1.89	0.54
1:A:372:SER:O	1:A:374:GLY:N	2.41	0.54
1:A:404:THR:HA	1:A:409:LEU:O	2.08	0.54
1:B:376:LYS:HG2	1:B:380:ASP:N	2.23	0.54
1:A:359:LEU:C	1:A:359:LEU:HD23	2.33	0.54
1:B:41:MET:O	1:B:459:PRO:HD3	2.08	0.54
1:B:155:PHE:HB2	1:B:160:ALA:HB2	1.89	0.53
1:B:192:SER:HB3	1:B:195:ASP:OD2	2.08	0.53
1:A:379:ARG:HG3	1:A:379:ARG:HH21	1.72	0.53
1:A:115:GLU:HA	1:A:115:GLU:OE2	2.07	0.53
1:A:297:VAL:HG13	1:A:298:ARG:N	2.23	0.53
1:B:29:GLU:OE1	1:B:33:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HD13	1:A:135:THR:HG21	1.91	0.52
1:B:278:LEU:HD13	1:B:306:HIS:NE2	2.25	0.52
1:B:304:PRO:HD2	1:B:306:HIS:H	1.73	0.52
1:B:416:GLU:N	1:B:416:GLU:OE1	2.43	0.52
1:A:52:LEU:HG	1:A:56:ILE:HD12	1.91	0.52
1:B:295:LYS:HG2	1:B:296:ASP:H	1.74	0.52
1:A:236:LYS:HA	1:A:243:TYR:CD1	2.45	0.51
1:B:278:LEU:HD13	1:B:306:HIS:CD2	2.44	0.51
1:A:208:VAL:HG13	1:A:215:ILE:HG22	1.91	0.51
1:A:208:VAL:HG12	1:A:215:ILE:HG23	1.89	0.51
1:B:49:LEU:HD13	1:B:106:VAL:HG21	1.92	0.51
1:B:303:GLY:HA2	1:B:307:ASP:OD2	2.10	0.51
1:B:380:ASP:CG	1:B:381:CYS:H	2.19	0.51
1:A:169:VAL:O	1:A:173:VAL:HG23	2.10	0.51
1:B:412:ASP:OD2	1:B:413:ALA:N	2.44	0.51
1:A:277:ARG:HD2	1:A:298:ARG:O	2.10	0.51
1:B:229:ARG:HH11	1:B:229:ARG:HA	1.75	0.51
1:B:249:LEU:HA	1:B:257:SER:OG	2.10	0.51
1:A:116:ASN:CG	1:A:117:LEU:H	2.16	0.51
1:B:232:TYR:OH	1:B:262:ILE:O	2.20	0.51
1:B:35:LEU:O	1:B:36:ASP:CA	2.47	0.51
1:B:180:ASP:OD1	1:B:180:ASP:O	2.29	0.51
1:B:198:PHE:HE2	1:B:462:LEU:CD2	2.24	0.51
1:A:41:MET:HB3	1:A:457:TRP:O	2.10	0.50
1:B:225:GLU:OE1	1:B:225:GLU:HA	2.11	0.50
1:A:295:LYS:O	1:A:296:ASP:OD1	2.30	0.50
1:A:305:GLY:C	1:A:307:ASP:N	2.69	0.50
1:A:464:ALA:O	1:A:465:ASP:HB2	2.11	0.50
1:B:298:ARG:O	1:B:299:LYS:C	2.53	0.50
1:B:335:ARG:HH12	1:B:407:SER:CB	2.23	0.50
1:A:14:MET:HE1	1:A:55:GLN:NE2	2.27	0.50
1:A:145:GLU:OE1	1:A:145:GLU:CA	2.54	0.50
1:A:154:TYR:O	1:A:155:PHE:O	2.29	0.50
1:A:237:SER:O	1:A:238:GLU:O	2.30	0.50
1:A:126:ILE:HG21	1:A:189:PHE:HZ	1.77	0.50
1:B:41:MET:HB3	1:B:457:TRP:O	2.12	0.50
1:A:238:GLU:HG3	1:A:239:PHE:CD2	2.46	0.50
1:B:393:ARG:NH1	1:B:417:ILE:HG21	2.27	0.50
1:A:341:ARG:HB2	1:A:341:ARG:NH1	2.23	0.49
1:A:453:ASP:N	1:A:454:THR:N	2.58	0.49
1:B:285:LEU:HD13	1:B:346:ILE:HG21	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:O	1:B:188:GLY:HA3	2.13	0.49
1:B:277:ARG:CD	1:B:298:ARG:O	2.48	0.49
1:B:294:LEU:O	1:B:295:LYS:O	2.29	0.49
1:B:395:ARG:HH21	1:B:413:ALA:HA	1.76	0.49
1:A:272:TYR:O	1:A:298:ARG:NH1	2.45	0.49
1:A:175:LYS:HD2	1:A:409:LEU:HD23	1.94	0.48
1:B:372:SER:C	1:B:374:GLY:N	2.70	0.48
1:B:387:ILE:O	1:B:387:ILE:CG1	2.60	0.48
1:A:238:GLU:O	1:A:239:PHE:CB	2.62	0.48
1:A:305:GLY:O	1:A:307:ASP:N	2.46	0.48
1:B:290:GLU:C	1:B:292:TRP:H	2.21	0.48
1:B:301:LYS:CG	1:B:302:LEU:H	2.24	0.48
1:A:324:TYR:CE2	1:A:341:ARG:HD3	2.48	0.48
1:A:453:ASP:CB	1:A:454:THR:N	2.76	0.48
1:B:246:TYR:CE1	1:B:419:VAL:HG13	2.49	0.48
1:A:110:THR:O	1:A:111:ARG:C	2.56	0.48
1:A:232:TYR:OH	1:A:262:ILE:O	2.23	0.48
1:A:237:SER:O	1:A:237:SER:OG	2.30	0.47
1:A:324:TYR:CE2	1:A:341:ARG:CD	2.97	0.47
1:B:387:ILE:HD11	1:B:424:THR:HG1	1.74	0.47
1:A:28:THR:HG22	1:A:29:GLU:H	1.79	0.47
1:A:296:ASP:OD2	1:A:297:VAL:N	2.40	0.47
1:B:391:PHE:HB2	1:B:420:ALA:HB3	1.97	0.47
1:A:176:LEU:HB3	1:A:338:ILE:HD12	1.95	0.47
1:A:273:VAL:HG11	1:A:279:PRO:HB3	1.95	0.47
1:A:372:SER:C	1:A:374:GLY:N	2.73	0.47
1:B:145:GLU:OE1	1:B:145:GLU:CA	2.62	0.47
1:B:206:VAL:O	1:B:207:ASN:HB2	2.13	0.47
1:B:105:TYR:O	1:B:109:MET:HB2	2.15	0.47
1:B:142:LYS:CD	1:B:142:LYS:N	2.69	0.47
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.73	0.47
1:A:370:ARG:HE	1:A:370:ARG:HB2	1.40	0.46
1:A:297:VAL:CG1	1:A:298:ARG:N	2.72	0.46
1:B:140:PRO:HG3	1:B:443:SER:O	2.15	0.46
1:B:412:ASP:OD2	1:B:412:ASP:C	2.59	0.46
1:B:444:TRP:O	1:B:445:LYS:C	2.57	0.46
1:B:41:MET:HE2	1:B:444:TRP:CH2	2.51	0.46
1:B:33:ARG:NE	1:B:33:ARG:HA	2.31	0.46
1:B:273:VAL:HG11	1:B:279:PRO:HB3	1.97	0.46
1:A:103:CYS:HB3	1:A:368:TYR:OH	2.15	0.46
1:B:198:PHE:HE2	1:B:462:LEU:HD23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:THR:OG1	1:B:98:GLN:HG3	2.16	0.46
1:A:324:TYR:HB3	1:A:326:MET:CE	2.47	0.45
1:B:253:PRO:O	1:B:254:CYS:HB3	2.16	0.45
1:B:341:ARG:O	1:B:341:ARG:CG	2.64	0.45
1:B:443:SER:O	1:B:446:ALA:HB3	2.17	0.45
1:A:46:PHE:HE1	1:A:99:ARG:HG2	1.80	0.45
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.65	0.45
1:B:19:PHE:O	1:B:20:ALA:C	2.59	0.45
1:B:256:ARG:HH11	1:B:256:ARG:CG	1.95	0.45
1:A:377:PRO:HD3	1:B:384:ARG:HH12	1.81	0.45
1:B:57:GLN:NE2	1:B:63:THR:HB	2.32	0.45
1:B:207:ASN:ND2	1:B:220:ARG:O	2.29	0.45
1:B:296:ASP:OD2	1:B:296:ASP:C	2.59	0.45
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.77	0.45
1:B:111:ARG:NH1	1:B:213:ASP:O	2.43	0.45
1:A:290:GLU:C	1:A:292:TRP:N	2.73	0.45
1:B:14:MET:HE1	1:B:55:GLN:CD	2.41	0.45
1:B:227:LYS:HG2	1:B:354:TYR:CE1	2.52	0.45
1:A:447:TYR:C	1:A:447:TYR:CD2	2.94	0.45
1:A:273:VAL:O	1:A:288:GLN:HG2	2.16	0.44
1:B:380:ASP:CG	1:B:381:CYS:N	2.73	0.44
1:B:375:GLY:C	1:B:376:LYS:CE	2.89	0.44
1:B:384:ARG:CG	1:B:384:ARG:NH1	2.59	0.44
1:B:447:TYR:O	1:B:448:ALA:C	2.60	0.44
1:B:111:ARG:HA	1:B:188:GLY:CA	2.48	0.44
1:B:387:ILE:CD1	1:B:387:ILE:C	2.83	0.44
1:B:440:ALA:O	1:B:443:SER:HB3	2.17	0.44
1:A:301:LYS:O	1:A:301:LYS:CD	2.66	0.44
1:B:209:GLU:OE2	1:B:218:THR:HG21	2.17	0.44
1:A:372:SER:C	1:A:374:GLY:H	2.26	0.44
1:B:301:LYS:CB	1:B:301:LYS:HZ3	2.31	0.44
1:B:302:LEU:HB3	1:B:303:GLY:H	1.58	0.44
1:B:376:LYS:HG2	1:B:380:ASP:O	2.18	0.44
1:A:114:SER:HA	1:A:119:TRP:CE3	2.52	0.43
1:A:149:ILE:CD1	1:A:151:THR:HG23	2.48	0.43
1:A:380:ASP:OD2	1:A:380:ASP:C	2.61	0.43
1:B:224:TYR:CD2	1:B:386:ASN:HB2	2.53	0.43
1:A:240:ASP:HA	1:A:241:PRO:HD3	1.75	0.43
1:A:147:ALA:HA	1:A:148:PRO:HD2	1.67	0.43
1:B:350:PRO:HA	1:B:355:PHE:CG	2.53	0.43
1:A:38:PRO:CB	1:A:457:TRP:HD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:O	1:A:292:TRP:N	2.52	0.43
1:A:350:PRO:HA	1:A:355:PHE:CG	2.53	0.43
1:B:273:VAL:O	1:B:288:GLN:HG2	2.18	0.43
1:A:237:SER:C	1:A:238:GLU:O	2.59	0.43
1:A:302:LEU:HD22	1:A:302:LEU:HA	1.78	0.43
1:B:159:VAL:O	1:B:163:LEU:HG	2.18	0.43
1:A:140:PRO:HG2	1:A:447:TYR:CB	2.48	0.43
1:A:33:ARG:HA	1:A:33:ARG:HE	1.81	0.43
1:A:37:ARG:HH22	1:B:327:THR:HG22	1.84	0.43
1:A:301:LYS:HE2	1:A:302:LEU:CD2	2.49	0.43
1:A:229:ARG:HA	1:A:229:ARG:HH11	1.83	0.43
1:A:460:SER:HB2	1:A:463:PHE:CD2	2.54	0.43
1:B:447:TYR:C	1:B:447:TYR:CD2	2.96	0.42
1:A:25:SER:HB3	1:A:27:GLU:HG2	2.00	0.42
1:A:294:LEU:O	1:A:295:LYS:CG	2.67	0.42
1:A:417:ILE:HA	1:A:418:PRO:HD2	1.96	0.42
1:B:359:LEU:HD23	1:B:360:LEU:N	2.34	0.42
1:A:137:LYS:HB2	1:A:137:LYS:HE3	1.73	0.42
1:B:217:PHE:HB3	1:B:369:VAL:HG22	2.02	0.42
1:B:262:ILE:HD13	1:B:262:ILE:HA	1.76	0.42
1:B:38:PRO:HB2	1:B:457:TRP:HD1	1.84	0.42
1:B:111:ARG:HA	1:B:188:GLY:HA2	2.01	0.42
1:B:180:ASP:OD1	1:B:180:ASP:N	2.47	0.42
1:B:301:LYS:HZ2	1:B:301:LYS:HG3	1.34	0.42
1:A:207:ASN:HB2	1:A:220:ARG:O	2.20	0.42
1:A:236:LYS:HA	1:A:243:TYR:CE1	2.55	0.42
1:B:273:VAL:HA	1:B:274:PRO:HD3	1.66	0.42
1:A:37:ARG:O	1:A:38:PRO:C	2.63	0.42
1:A:200:VAL:HB	1:A:364:ILE:HD12	2.02	0.42
1:A:284:TYR:O	1:A:348:ILE:HD12	2.20	0.42
1:A:198:PHE:HE2	1:A:462:LEU:HD13	1.85	0.42
1:A:324:TYR:HB3	1:A:326:MET:HE1	2.02	0.42
1:B:273:VAL:HG23	1:B:277:ARG:HB2	2.01	0.42
1:A:377:PRO:HD3	1:B:384:ARG:HH22	1.85	0.41
1:B:404:THR:CA	1:B:409:LEU:O	2.65	0.41
1:A:32:VAL:HA	1:A:35:LEU:HG	2.02	0.41
1:A:57:GLN:NE2	1:A:63:THR:HG22	2.19	0.41
1:A:113:GLN:H	1:A:113:GLN:HG3	1.51	0.41
1:A:354:TYR:N	1:A:354:TYR:CD2	2.86	0.41
1:B:211:GLN:HE21	1:B:211:GLN:HB3	1.58	0.41
1:A:444:TRP:O	1:A:445:LYS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:HG11	1:B:86:SER:O	2.21	0.41
1:A:246:TYR:CE1	1:A:419:VAL:HG13	2.56	0.41
1:B:133:LEU:HD13	1:B:356:TYR:CE1	2.56	0.41
1:B:269:THR:HA	1:B:283:ASP:OD2	2.20	0.41
1:A:261:PHE:O	1:A:262:ILE:C	2.61	0.41
1:B:290:GLU:C	1:B:292:TRP:N	2.79	0.41
1:A:95:THR:OG1	1:A:98:GLN:HG3	2.21	0.41
1:B:97:GLU:O	1:B:101:VAL:HG23	2.20	0.41
1:B:328:ASP:HA	1:B:329:PRO:HD2	1.89	0.41
1:B:395:ARG:NH2	1:B:413:ALA:HA	2.35	0.41
1:B:100:THR:HG21	1:B:371:HIS:HB2	2.02	0.41
1:B:256:ARG:NH1	1:B:256:ARG:CG	2.65	0.40
1:A:161:PHE:CE2	1:A:228:CYS:HB3	2.56	0.40
1:B:50:TYR:CZ	1:B:87:ILE:CD1	3.04	0.40
1:B:277:ARG:HD3	1:B:300:ARG:HA	2.03	0.40
1:B:117:LEU:O	1:B:121:ILE:HG13	2.21	0.40
1:A:198:PHE:HE2	1:A:462:LEU:CD1	2.35	0.40
1:A:273:VAL:HA	1:A:274:PRO:HD3	1.72	0.40
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.82	0.40
1:B:200:VAL:HB	1:B:364:ILE:HD12	2.02	0.40

All (5) 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:341:ARG:NH1	1:B:36:ASP:O[2_645]	1.69	0.51
1:A:58:GLU:OE2	1:A:156:GLY:N[2_656]	1.72	0.48
1:A:58:GLU:OE2	1:A:156:GLY:CA[2_656]	1.81	0.39
1:A:58:GLU:OE2	1:A:156:GLY:C[2_656]	1.94	0.26
1:A:58:GLU:OE2	1:A:157:GLY:N[2_656]	2.17	0.03

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	452/470 (96%)	370 (82%)	65 (14%)	17 (4%)	2	20
1	B	431/470 (92%)	369 (86%)	46 (11%)	16 (4%)	2	21
All	All	883/940 (94%)	739 (84%)	111 (13%)	33 (4%)	2	21

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	42	PRO
1	A	148	PRO
1	A	295	LYS
1	A	296	ASP
1	A	304	PRO
1	A	465	ASP
1	B	114	SER
1	B	295	LYS
1	B	296	ASP
1	B	304	PRO
1	A	29	GLU
1	A	152	ASN
1	A	155	PHE
1	A	280	SER
1	A	303	GLY
1	A	373	GLY
1	B	42	PRO
1	B	373	GLY
1	B	381	CYS
1	A	306	HIS
1	B	280	SER
1	B	291	ALA
1	B	166	GLU
1	B	408	ASP
1	A	153	HIS
1	B	319	VAL
1	A	238	GLU
1	B	168	THR
1	B	374	GLY
1	B	305	GLY
1	A	179	GLY
1	B	282	GLY

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	400/414 (97%)	325 (81%)	75 (19%)	1	9
1	B	386/414 (93%)	317 (82%)	69 (18%)	2	10
All	All	786/828 (95%)	642 (82%)	144 (18%)	2	10

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	GLU
1	A	21	ARG
1	A	23	LEU
1	A	28	THR
1	A	33	ARG
1	A	37	ARG
1	A	44	MET
1	A	62	GLU
1	A	74	GLN
1	A	86	SER
1	A	100	THR
1	A	113	GLN
1	A	115	GLU
1	A	120	ASP
1	A	126	ILE
1	A	130	SER
1	A	135	THR
1	A	136	ILE
1	A	141	THR
1	A	142	LYS
1	A	143	VAL
1	A	145	GLU
1	A	151	THR
1	A	166	GLU
1	A	178	CYS
1	A	180	ASP

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Mol	Chain	Res	Type
1	A	200	VAL
1	A	203	SER
1	A	210	SER
1	A	218	THR
1	A	225	GLU
1	A	229	ARG
1	A	233	LEU
1	A	237	SER
1	A	247	THR
1	A	252	ARG
1	A	255	LYS
1	A	256	ARG
1	A	262	ILE
1	A	267	ARG
1	A	273	VAL
1	A	278	LEU
1	A	294	LEU
1	A	295	LYS
1	A	296	ASP
1	A	297	VAL
1	A	298	ARG
1	A	301	LYS
1	A	302	LEU
1	A	309	VAL
1	A	316	ASN
1	A	317	ARG
1	A	339	LYS
1	A	341	ARG
1	A	344	VAL
1	A	358	VAL
1	A	359	LEU
1	A	376	LYS
1	A	380	ASP
1	A	384	ARG
1	A	385	VAL
1	A	402	THR
1	A	407	SER
1	A	409	LEU
1	A	410	LEU
1	A	419	VAL
1	A	423	VAL
1	A	435	LYS

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Mol	Chain	Res	Type
1	A	439	THR
1	A	447	TYR
1	A	454	THR
1	A	457	TRP
1	A	462	LEU
1	A	466	ASP
1	B	21	ARG
1	B	23	LEU
1	B	24	ARG
1	B	27	GLU
1	B	28	THR
1	B	33	ARG
1	B	54	LYS
1	B	62	GLU
1	B	74	GLN
1	B	86	SER
1	B	100	THR
1	B	113	GLN
1	B	115	GLU
1	B	116	ASN
1	B	120	ASP
1	B	126	ILE
1	B	135	THR
1	B	141	THR
1	B	142	LYS
1	B	143	VAL
1	B	155	PHE
1	B	166	GLU
1	B	200	VAL
1	B	203	SER
1	B	220	ARG
1	B	222	CYS
1	B	225	GLU
1	B	229	ARG
1	B	237	SER
1	B	247	THR
1	B	251	LYS
1	B	252	ARG
1	B	255	LYS
1	B	256	ARG
1	B	262	ILE
1	B	267	ARG

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Mol	Chain	Res	Type
1	B	273	VAL
1	B	278	LEU
1	B	294	LEU
1	B	297	VAL
1	B	298	ARG
1	B	301	LYS
1	B	302	LEU
1	B	309	VAL
1	B	316	ASN
1	B	317	ARG
1	B	320	GLU
1	B	339	LYS
1	B	341	ARG
1	B	344	VAL
1	B	358	VAL
1	B	359	LEU
1	B	370	ARG
1	B	376	LYS
1	B	384	ARG
1	B	385	VAL
1	B	402	THR
1	B	407	SER
1	B	409	LEU
1	B	410	LEU
1	B	415	VAL
1	B	419	VAL
1	B	423	VAL
1	B	434	ARG
1	B	435	LYS
1	B	439	THR
1	B	447	TYR
1	B	454	THR
1	B	457	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	57	GLN
1	A	74	GLN
1	A	92	GLN
1	A	316	ASN

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Mol	Chain	Res	Type
1	A	353	ASN
1	A	386	ASN
1	A	450	ASN
1	B	34	ASN
1	B	40	GLN
1	B	55	GLN
1	B	74	GLN
1	B	92	GLN
1	B	288	GLN
1	B	316	ASN
1	B	332	ASN
1	B	353	ASN
1	B	371	HIS
1	B	386	ASN
1	B	450	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:ASP	C	37:ARG	N	1.13
1	B	36:ASP	C	37:ARG	N	1.07
1	B	35:LEU	C	36:ASP	N	0.85
1	A	453:ASP	C	454:THR	N	0.80
1	A	452:PHE	C	453:ASP	N	0.40

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	456/470 (97%)	1.12	64 (14%) 6 5	28, 44, 73, 91	0
1	B	439/470 (93%)	0.80	38 (8%) 16 10	25, 43, 66, 85	0
All	All	895/940 (95%)	0.96	102 (11%) 10 7	25, 43, 70, 91	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	TYR	6.8
1	A	30	ALA	5.1
1	A	180	ASP	5.0
1	B	304	PRO	4.7
1	A	36	ASP	4.4
1	A	28	THR	4.3
1	A	296	ASP	4.2
1	A	153	HIS	4.2
1	A	181	ALA	4.2
1	A	183	ALA	4.1
1	A	58	GLU	4.1
1	A	31	PHE	4.0
1	A	304	PRO	3.8
1	A	27	GLU	3.8
1	A	149	ILE	3.8
1	B	406	GLY	3.7
1	B	62	GLU	3.6
1	B	306	HIS	3.5
1	B	302	LEU	3.4
1	B	300	ARG	3.4
1	A	150	SER	3.3
1	A	467	GLU	3.3
1	A	375	GLY	3.3
1	A	454	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	58	GLU	3.1
1	A	274	PRO	3.1
1	A	297	VAL	3.1
1	A	466	ASP	3.0
1	A	156	GLY	3.0
1	B	299	LYS	3.0
1	A	26	PRO	2.9
1	A	29	GLU	2.9
1	B	89	TRP	2.9
1	A	306	HIS	2.9
1	A	151	THR	2.9
1	B	156	GLY	2.8
1	A	457	TRP	2.8
1	B	380	ASP	2.8
1	B	307	ASP	2.7
1	A	184	ASN	2.7
1	B	60	SER	2.7
1	B	305	GLY	2.7
1	A	7	LEU	2.6
1	A	330	SER	2.6
1	A	277	ARG	2.6
1	B	182	SER	2.6
1	A	414	SER	2.6
1	A	73	VAL	2.6
1	B	372	SER	2.5
1	A	118	MET	2.5
1	A	450	ASN	2.5
1	B	408	ASP	2.5
1	A	182	SER	2.5
1	A	300	ARG	2.5
1	A	146	PRO	2.5
1	A	302	LEU	2.5
1	B	303	GLY	2.5
1	A	148	PRO	2.4
1	A	108	SER	2.4
1	A	155	PHE	2.4
1	A	62	GLU	2.4
1	B	298	ARG	2.4
1	A	303	GLY	2.4
1	B	294	LEU	2.4
1	B	146	PRO	2.4
1	A	59	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	84	LEU	2.4
1	A	147	ALA	2.4
1	A	448	ALA	2.4
1	B	375	GLY	2.3
1	A	116	ASN	2.3
1	A	12	GLU	2.3
1	A	374	GLY	2.3
1	B	374	GLY	2.3
1	B	463	PHE	2.3
1	B	297	VAL	2.3
1	A	37	ARG	2.2
1	A	279	PRO	2.2
1	B	183	ALA	2.2
1	B	157	GLY	2.2
1	A	43	ALA	2.2
1	B	437	LEU	2.2
1	A	10	PRO	2.2
1	A	410	LEU	2.2
1	B	381	CYS	2.1
1	B	295	LYS	2.1
1	B	376	LYS	2.1
1	A	117	LEU	2.1
1	A	179	GLY	2.1
1	B	26	PRO	2.1
1	B	459	PRO	2.1
1	A	87	ILE	2.1
1	A	186	GLN	2.1
1	B	9	ASP	2.1
1	A	208	VAL	2.1
1	A	446	ALA	2.1
1	B	340	ASP	2.1
1	B	341	ARG	2.0
1	A	247	THR	2.0
1	B	462	LEU	2.0
1	A	18	THR	2.0
1	B	75	GLU	2.0

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

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.