



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:31 AM UTC

PDB ID : 2FRX / pdb_00002frx
Title : Crystal structure of YebU, a m5C RNA methyltransferase from E.coli
Authors : Erlandsen, H.; Nordlund, P.; Hallberg, B.M.; Johnson, K.A.; Ericsson, U.B.
Deposited on : 2006-01-20
Resolution : 2.90 Å(reported)

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

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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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

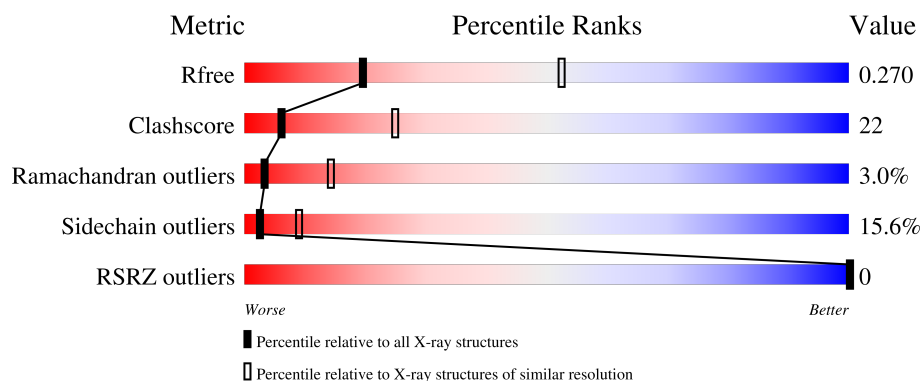
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	479	
1	B	479	
1	C	479	
1	D	479	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14266 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 Hypothetical protein yebU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	Se	0	0	0
			3574	2285	621	654	7	7			
1	B	454	Total	C	N	O	S	Se	0	0	0
			3562	2276	620	652	7	7			
1	C	454	Total	C	N	O	S	Se	0	0	0
			3562	2276	620	652	7	7			
1	D	455	Total	C	N	O	S	Se	0	0	0
			3568	2282	618	654	7	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P76273
A	16	MSE	MET	modified residue	UNP P76273
A	20	MSE	MET	modified residue	UNP P76273
A	105	MSE	MET	modified residue	UNP P76273
A	122	MSE	MET	modified residue	UNP P76273
A	139	MSE	MET	modified residue	UNP P76273
A	187	MSE	MET	modified residue	UNP P76273
A	411	MSE	MET	modified residue	UNP P76273
B	1	MSE	MET	modified residue	UNP P76273
B	16	MSE	MET	modified residue	UNP P76273
B	20	MSE	MET	modified residue	UNP P76273
B	105	MSE	MET	modified residue	UNP P76273
B	122	MSE	MET	modified residue	UNP P76273
B	139	MSE	MET	modified residue	UNP P76273
B	187	MSE	MET	modified residue	UNP P76273
B	411	MSE	MET	modified residue	UNP P76273
C	1	MSE	MET	modified residue	UNP P76273
C	16	MSE	MET	modified residue	UNP P76273
C	20	MSE	MET	modified residue	UNP P76273
C	105	MSE	MET	modified residue	UNP P76273
C	122	MSE	MET	modified residue	UNP P76273

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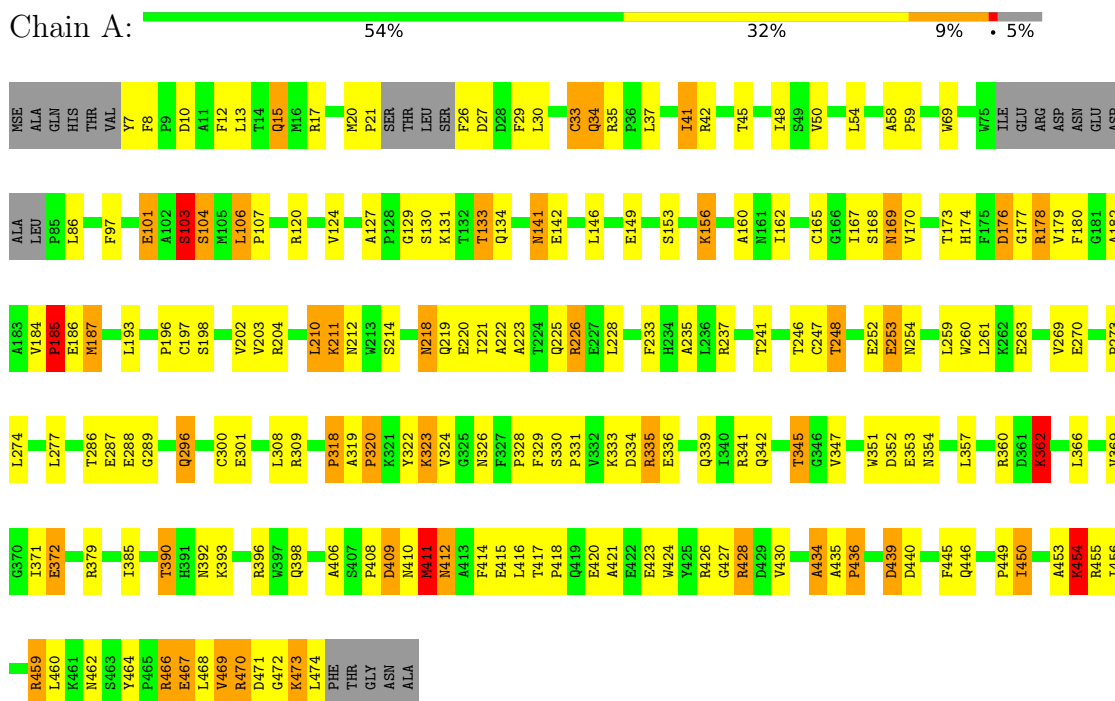
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Chain	Residue	Modelled	Actual	Comment	Reference
C	139	MSE	MET	modified residue	UNP P76273
C	187	MSE	MET	modified residue	UNP P76273
C	411	MSE	MET	modified residue	UNP P76273
D	1	MSE	MET	modified residue	UNP P76273
D	16	MSE	MET	modified residue	UNP P76273
D	20	MSE	MET	modified residue	UNP P76273
D	105	MSE	MET	modified residue	UNP P76273
D	122	MSE	MET	modified residue	UNP P76273
D	139	MSE	MET	modified residue	UNP P76273
D	187	MSE	MET	modified residue	UNP P76273
D	411	MSE	MET	modified residue	UNP P76273

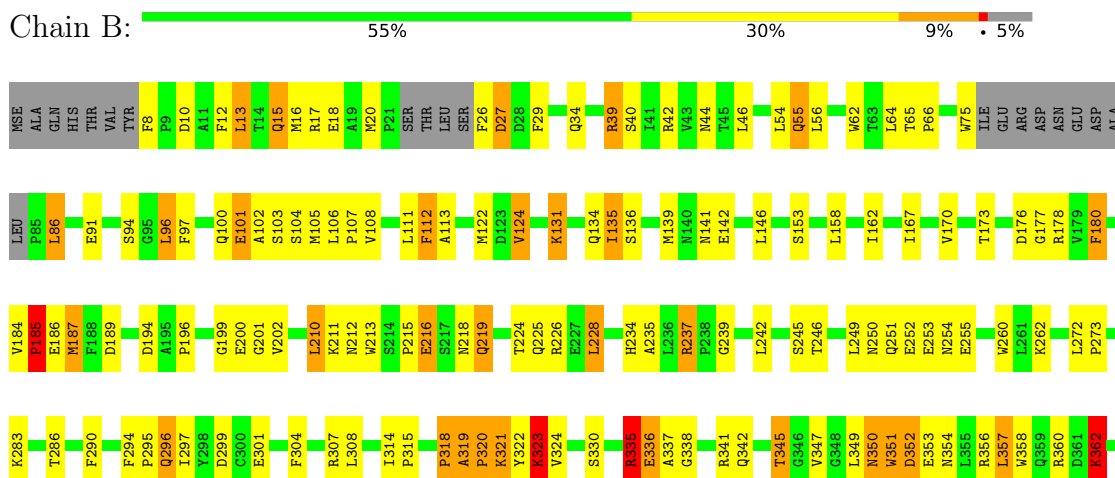
3 Residue-property plots

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: Hypothetical protein yebU



• Molecule 1: Hypothetical protein yebU



Y431	D439	D440	V441	V442	V443	T444	F445	Q446	H447	Q448	P449	I450	G451	L452	A453	K454	R455	I456	G457	S458	R459	L460	K461	N462	S463	Y464	F465	R466	E467	L468	V469	R470	D471	G472	R473	L474	PHE	THR	GLY	ASN	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.71Å 87.13Å 95.05Å 88.33° 76.79° 90.19°	Depositor
Resolution (Å)	29.03 – 2.90 29.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.03-2.90) 89.5 (29.03-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.231 , 0.282 0.216 , 0.270	Depositor DCC
R_{free} test set	2314 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.093 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14266	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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	1.02	14/3659 (0.4%)	1.16	12/4963 (0.2%)
1	B	1.07	7/3646 (0.2%)	1.20	10/4945 (0.2%)
1	C	1.19	14/3646 (0.4%)	1.20	6/4945 (0.1%)
1	D	1.61	39/3653 (1.1%)	1.22	21/4956 (0.4%)
All	All	1.24	74/14604 (0.5%)	1.20	49/19809 (0.2%)

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
1	C	0	1
1	D	0	2
All	All	0	6

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	335	ARG	NE-CZ	46.84	1.84	1.33
1	D	459	ARG	NE-CZ	26.05	1.61	1.33
1	D	420	GLU	CD-OE1	22.57	1.68	1.25
1	C	214	SER	CB-OG	21.54	1.85	1.42
1	C	428	ARG	CZ-NH1	19.70	1.60	1.32
1	D	10	ASP	CG-OD2	19.52	1.62	1.25
1	D	10	ASP	CG-OD1	16.24	1.56	1.25
1	D	17	ARG	NE-CZ	15.81	1.50	1.33
1	D	17	ARG	CD-NE	13.61	1.65	1.46
1	D	428	ARG	CZ-NH1	13.45	1.51	1.32
1	D	428	ARG	NE-CZ	12.93	1.47	1.33
1	C	428	ARG	CD-NE	12.60	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	ARG	CZ-NH1	11.62	1.49	1.32
1	C	428	ARG	CZ-NH2	11.38	1.48	1.33
1	C	428	ARG	NE-CZ	11.38	1.45	1.33
1	D	208	ASP	CG-OD1	11.10	1.46	1.25
1	D	420	GLU	CD-OE2	10.61	1.45	1.25
1	A	335	ARG	NE-CZ	10.40	1.44	1.33
1	D	431	TYR	CE1-CZ	10.21	1.62	1.38
1	D	208	ASP	CG-OD2	9.97	1.44	1.25
1	A	454	LYS	CE-NZ	9.85	1.78	1.49
1	C	411	MSE	SE-CE	9.21	2.23	1.95
1	D	17	ARG	CZ-NH2	-8.90	1.21	1.33
1	B	411	MSE	SE-CE	8.82	2.21	1.95
1	D	17	ARG	CZ-NH1	8.64	1.44	1.32
1	D	439	ASP	CG-OD1	8.49	1.41	1.25
1	A	17	ARG	NE-CZ	8.47	1.42	1.33
1	D	339	GLN	CD-OE1	8.47	1.39	1.23
1	A	27	ASP	CG-OD2	8.18	1.40	1.25
1	D	187	MSE	SE-CE	7.96	2.19	1.95
1	A	10	ASP	CG-OD2	7.95	1.40	1.25
1	A	27	ASP	CG-OD1	7.87	1.40	1.25
1	B	34	GLN	CD-OE1	7.58	1.38	1.23
1	B	187	MSE	SE-CE	7.48	2.17	1.95
1	C	187	MSE	SE-CE	7.46	2.17	1.95
1	D	433	GLN	CD-OE1	7.44	1.37	1.23
1	D	431	TYR	CG-CD2	7.40	1.54	1.39
1	D	28	ASP	CG-OD2	7.33	1.39	1.25
1	D	431	TYR	CG-CD1	7.27	1.54	1.39
1	D	459	ARG	CG-CD	6.97	1.73	1.52
1	D	428	ARG	CZ-NH2	6.74	1.42	1.33
1	A	187	MSE	SE-CE	6.73	2.15	1.95
1	D	473	LYS	CE-NZ	6.52	1.69	1.49
1	D	214	SER	CB-OG	6.37	1.54	1.42
1	A	411	MSE	SE-CE	6.35	2.14	1.95
1	D	18	GLU	CD-OE1	6.31	1.37	1.25
1	C	216	GLU	CD-OE2	6.29	1.37	1.25
1	A	10	ASP	CG-OD1	6.17	1.37	1.25
1	A	428	ARG	CZ-NH1	6.17	1.41	1.32
1	B	10	ASP	CG-OD1	6.09	1.36	1.25
1	C	216	GLU	CD-OE1	6.04	1.36	1.25
1	C	105	MSE	SE-CE	5.89	2.13	1.95
1	D	18	GLU	CD-OE2	5.85	1.36	1.25
1	B	10	ASP	CG-OD2	5.84	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	ARG	CD-NE	5.84	1.54	1.46
1	A	454	LYS	CD-CE	5.83	1.70	1.52
1	D	283	LYS	CD-CE	5.82	1.69	1.52
1	A	392	ASN	CG-OD1	5.81	1.34	1.23
1	D	206	ASP	CG-OD1	5.77	1.36	1.25
1	C	20	MSE	SE-CE	5.71	2.12	1.95
1	D	428	ARG	CD-NE	5.66	1.54	1.46
1	D	26	PHE	CG-CD2	5.64	1.50	1.38
1	D	439	ASP	CG-OD2	5.64	1.36	1.25
1	D	28	ASP	CG-OD1	5.62	1.36	1.25
1	A	133	THR	CA-CB	5.59	1.62	1.53
1	D	243	VAL	CA-CB	5.58	1.60	1.54
1	A	17	ARG	CD-NE	5.51	1.53	1.46
1	D	335	ARG	CZ-NH2	5.27	1.40	1.33
1	B	18	GLU	CD-OE1	5.26	1.35	1.25
1	B	319	ALA	CA-CB	5.21	1.61	1.53
1	D	14	THR	CA-CB	5.13	1.62	1.53
1	C	10	ASP	CG-OD2	5.11	1.35	1.25
1	D	333	LYS	CE-NZ	5.09	1.64	1.49
1	D	458	SER	CB-OG	5.05	1.52	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	428	ARG	NE-CZ-NH2	-15.99	104.81	119.20
1	D	17	ARG	NE-CZ-NH2	13.89	131.70	119.20
1	C	428	ARG	NE-CZ-NH1	13.84	135.34	121.50
1	C	428	ARG	CD-NE-CZ	-11.23	108.68	124.40
1	D	459	ARG	NE-CZ-NH2	-9.61	110.55	119.20
1	D	335	ARG	NE-CZ-NH2	-9.57	110.59	119.20
1	D	428	ARG	NE-CZ-NH2	-8.62	111.44	119.20
1	D	339	GLN	OE1-CD-NE2	7.28	129.88	122.60
1	D	17	ARG	NH1-CZ-NH2	-7.02	110.17	119.30
1	B	352	ASP	CB-CA-C	-6.49	97.23	111.71
1	D	187	MSE	N-CA-C	6.43	119.60	111.69
1	A	459	ARG	N-CA-C	6.24	121.56	113.88
1	D	420	GLU	CG-CD-OE1	-6.13	104.31	118.40
1	B	362	LYS	N-CA-C	-6.06	105.74	113.01
1	A	187	MSE	N-CA-C	5.92	118.97	111.69
1	D	459	ARG	N-CA-C	5.91	121.37	114.04
1	D	345	THR	N-CA-C	-5.86	104.89	111.28
1	A	50	VAL	CB-CA-C	-5.86	104.49	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	ILE	CB-CA-C	5.81	116.45	110.70
1	D	334	ASP	N-CA-C	5.80	117.69	111.36
1	C	184	VAL	CA-C-N	5.75	127.02	119.84
1	C	184	VAL	C-N-CA	5.75	127.02	119.84
1	A	326	ASN	N-CA-C	5.68	118.59	110.24
1	A	17	ARG	NE-CZ-NH1	5.65	127.15	121.50
1	A	362	LYS	N-CA-C	-5.58	106.31	113.01
1	D	326	ASN	N-CA-C	5.52	118.35	110.24
1	D	275	GLY	N-CA-C	5.51	121.05	113.99
1	D	276	ASP	CB-CA-C	-5.48	100.93	110.09
1	D	180	PHE	N-CA-C	5.48	117.68	111.11
1	A	160	ALA	N-CA-C	-5.46	105.33	111.28
1	B	139	MSE	N-CA-C	-5.45	106.30	113.17
1	D	103	SER	N-CA-CB	-5.43	101.31	110.49
1	A	103	SER	N-CA-C	5.35	117.81	111.33
1	A	345	THR	N-CA-C	-5.33	105.47	111.28
1	D	283	LYS	CG-CD-CE	-5.28	99.15	111.30
1	A	454	LYS	CD-CE-NZ	-5.26	95.07	111.90
1	A	86	LEU	N-CA-C	5.25	117.42	111.11
1	A	334	ASP	N-CA-C	5.21	116.64	111.07
1	D	319	ALA	N-CA-C	5.20	121.31	109.81
1	C	180	PHE	N-CA-C	5.20	117.35	111.11
1	B	319	ALA	N-CA-C	5.19	121.29	109.81
1	D	86	LEU	N-CA-C	5.13	117.27	111.11
1	B	430	VAL	N-CA-C	5.13	115.87	108.48
1	B	180	PHE	N-CA-C	5.09	116.52	111.07
1	B	345	THR	N-CA-C	-5.08	105.74	111.28
1	B	124	VAL	N-CA-C	5.06	115.29	110.53
1	D	317	LEU	N-CA-C	-5.05	104.24	110.31
1	D	208	ASP	CB-CA-C	-5.02	101.11	109.55
1	B	323	LYS	CB-CA-C	5.01	115.97	109.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	PRO	Peptide
1	B	318	PRO	Peptide
1	B	323	LYS	Peptide
1	C	318	PRO	Peptide
1	D	318	PRO	Peptide
1	D	459	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	3574	0	3513	138	0
1	B	3562	0	3504	158	0
1	C	3562	0	3504	164	0
1	D	3568	0	3502	177	0
All	All	14266	0	14023	635	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 22.

All (635) 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:D:473:LYS:CE	1:D:473:LYS:NZ	1.68	1.54
1:A:187:MSE:SE	1:A:187:MSE:CE	2.15	1.45
1:A:411:MSE:SE	1:A:411:MSE:CE	2.14	1.45
1:A:454:LYS:CE	1:A:454:LYS:NZ	1.78	1.43
1:B:187:MSE:SE	1:B:187:MSE:CE	2.17	1.42
1:C:187:MSE:SE	1:C:187:MSE:CE	2.17	1.42
1:D:187:MSE:SE	1:D:187:MSE:CE	2.19	1.39
1:D:335:ARG:CZ	1:D:335:ARG:NE	1.84	1.38
1:C:411:MSE:SE	1:C:411:MSE:CE	2.23	1.36
1:B:411:MSE:SE	1:B:411:MSE:CE	2.21	1.35
1:D:420:GLU:OE1	1:D:420:GLU:CD	1.68	1.34
1:B:318:PRO:O	1:B:320:PRO:HD3	1.33	1.28
1:D:318:PRO:O	1:D:320:PRO:HD3	1.31	1.27
1:C:214:SER:OG	1:C:214:SER:CB	1.85	1.24
1:C:318:PRO:O	1:C:320:PRO:HD3	1.35	1.21
1:B:94:SER:HB3	1:B:450:ILE:HD11	1.28	1.14
1:C:29:PHE:HA	1:C:296:GLN:HG2	1.30	1.12
1:B:341:ARG:HG2	1:B:351:TRP:HZ2	1.01	1.09
1:B:122:MSE:HE1	1:B:180:PHE:CE2	1.88	1.09
1:B:341:ARG:HG2	1:B:351:TRP:CZ2	1.90	1.06
1:B:335:ARG:HH11	1:B:335:ARG:CG	1.72	1.02
1:B:335:ARG:HG3	1:B:335:ARG:NH1	1.62	1.02
1:A:318:PRO:O	1:A:320:PRO:HD3	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ARG:HB3	1:C:335:ARG:HH11	1.20	1.00
1:A:223:ALA:HA	1:A:226:ARG:NH1	1.78	0.97
1:C:108:VAL:HG11	1:C:134:GLN:HG2	1.46	0.96
1:B:94:SER:HB3	1:B:450:ILE:CD1	1.95	0.96
1:B:416:LEU:HD22	1:B:420:GLU:HB3	1.47	0.96
1:B:341:ARG:CG	1:B:351:TRP:HZ2	1.78	0.96
1:D:106:LEU:HB3	1:D:107:PRO:HD3	1.48	0.95
1:B:225:GLN:HE22	1:B:253:GLU:HB3	1.32	0.95
1:C:341:ARG:HD3	1:C:351:TRP:CH2	2.02	0.94
1:B:29:PHE:HA	1:B:296:GLN:HG2	1.47	0.94
1:B:335:ARG:HH11	1:B:335:ARG:HG3	0.81	0.94
1:D:318:PRO:O	1:D:320:PRO:CD	2.17	0.92
1:A:225:GLN:OE1	1:A:253:GLU:HG2	1.71	0.91
1:B:399:HIS:CE1	1:B:403:ILE:HD11	2.06	0.91
1:C:176:ASP:O	1:C:178:ARG:N	2.06	0.88
1:C:318:PRO:O	1:C:320:PRO:CD	2.21	0.88
1:C:352:ASP:HB3	1:C:354:ASN:H	1.39	0.88
1:C:236:LEU:HD11	1:C:240:GLY:HA3	1.56	0.87
1:D:318:PRO:C	1:D:320:PRO:HD3	1.98	0.87
1:A:352:ASP:HB3	1:A:354:ASN:H	1.40	0.86
1:D:226:ARG:NH1	1:D:226:ARG:HG3	1.88	0.86
1:B:425:TYR:OH	1:B:450:ILE:CD1	2.25	0.85
1:A:416:LEU:HD22	1:A:420:GLU:HB3	1.58	0.84
1:C:20:MSE:HE3	1:C:21:PRO:HD2	1.59	0.83
1:B:176:ASP:O	1:B:178:ARG:N	2.11	0.83
1:A:318:PRO:C	1:A:320:PRO:HD3	2.02	0.82
1:A:223:ALA:HA	1:A:226:ARG:HH11	1.43	0.82
1:D:176:ASP:O	1:D:178:ARG:N	2.13	0.82
1:B:318:PRO:O	1:B:320:PRO:CD	2.25	0.81
1:D:103:SER:HB2	1:D:301:GLU:OE2	1.81	0.81
1:D:226:ARG:HG3	1:D:226:ARG:HH11	1.42	0.81
1:D:324:VAL:HG12	1:D:379:ARG:HE	1.43	0.81
1:B:184:VAL:HG12	1:B:187:MSE:HB2	1.60	0.81
1:B:131:LYS:O	1:B:135:ILE:HG12	1.79	0.81
1:D:185:PRO:O	1:D:235:ALA:HA	1.81	0.81
1:B:16:MSE:HE1	1:B:249:LEU:HB2	1.63	0.80
1:C:341:ARG:HD3	1:C:351:TRP:HH2	1.45	0.80
1:C:210:LEU:O	1:C:212:ASN:N	2.15	0.80
1:C:223:ALA:HA	1:C:226:ARG:HH12	1.47	0.80
1:C:318:PRO:C	1:C:320:PRO:HD3	2.06	0.79
1:D:363:GLU:HG2	1:D:386:LYS:HE3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ASP:O	1:A:178:ARG:N	2.16	0.79
1:B:318:PRO:C	1:B:320:PRO:HD3	2.07	0.79
1:A:185:PRO:O	1:A:235:ALA:HA	1.83	0.79
1:B:367:PHE:CE1	1:B:383:LEU:HB2	2.17	0.79
1:A:410:ASN:OD1	1:A:412:ASN:N	2.16	0.78
1:B:352:ASP:HB2	1:B:354:ASN:H	1.49	0.77
1:C:185:PRO:O	1:C:235:ALA:HA	1.83	0.77
1:D:178:ARG:HG3	1:D:178:ARG:HH11	1.46	0.77
1:C:127:ALA:HB1	1:C:154:ARG:HG2	1.67	0.77
1:B:219:GLN:OE1	1:B:219:GLN:HA	1.84	0.77
1:D:122:MSE:CE	1:D:146:LEU:HD22	2.15	0.77
1:A:29:PHE:HA	1:A:296:GLN:HG2	1.66	0.77
1:C:26:PHE:O	1:C:29:PHE:HB3	1.84	0.76
1:D:351:TRP:HE3	1:D:352:ASP:O	1.67	0.76
1:A:221:ILE:O	1:A:225:GLN:HG3	1.86	0.76
1:D:429:ASP:OD1	1:D:461:LYS:HA	1.86	0.75
1:B:122:MSE:HE1	1:B:180:PHE:CZ	2.21	0.75
1:B:351:TRP:HE3	1:B:351:TRP:O	1.69	0.75
1:C:223:ALA:HA	1:C:226:ARG:NH1	2.02	0.75
1:B:466:ARG:HA	1:B:469:VAL:HG13	1.67	0.75
1:D:416:LEU:HD22	1:D:420:GLU:HB3	1.67	0.75
1:A:445:PHE:HB3	1:A:450:ILE:CD1	2.17	0.74
1:D:341:ARG:CG	1:D:351:TRP:HZ2	2.01	0.74
1:B:341:ARG:NH2	1:B:351:TRP:CH2	2.56	0.74
1:A:103:SER:HB2	1:A:301:GLU:OE1	1.87	0.74
1:A:219:GLN:OE1	1:A:219:GLN:HA	1.85	0.74
1:D:226:ARG:HH11	1:D:226:ARG:CG	2.01	0.73
1:C:246:THR:OG1	1:C:254:ASN:ND2	2.20	0.73
1:B:362:LYS:HD3	1:B:362:LYS:N	2.04	0.73
1:C:341:ARG:HB2	1:C:351:TRP:CZ2	2.24	0.73
1:D:127:ALA:HB2	1:D:149:GLU:HG3	1.70	0.73
1:A:197:CYS:HB2	1:A:248:THR:CG2	2.19	0.73
1:A:176:ASP:OD1	1:A:176:ASP:N	2.22	0.73
1:C:335:ARG:HH11	1:C:335:ARG:CB	2.01	0.73
1:D:153:SER:HA	1:D:156:LYS:HE3	1.71	0.72
1:D:225:GLN:HE22	1:D:253:GLU:HG2	1.54	0.72
1:D:341:ARG:HG2	1:D:351:TRP:CZ2	2.23	0.72
1:B:26:PHE:O	1:B:29:PHE:HB3	1.89	0.72
1:B:176:ASP:O	1:B:176:ASP:CG	2.32	0.72
1:D:270:GLU:OE1	1:D:309:ARG:NH1	2.22	0.72
1:B:425:TYR:OH	1:B:450:ILE:HD13	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:PHE:CE2	1:D:176:ASP:HB3	2.25	0.72
1:D:29:PHE:HA	1:D:296:GLN:CG	2.19	0.72
1:B:210:LEU:O	1:B:212:ASN:N	2.22	0.71
1:C:367:PHE:CE1	1:C:383:LEU:HB2	2.25	0.71
1:B:108:VAL:HG11	1:B:134:GLN:HG2	1.73	0.71
1:C:338:GLY:HA2	1:C:341:ARG:NH2	2.06	0.71
1:A:473:LYS:NZ	1:A:473:LYS:H	1.89	0.71
1:D:106:LEU:HB3	1:D:107:PRO:CD	2.19	0.70
1:D:150:PHE:HE2	1:D:176:ASP:HB3	1.55	0.70
1:C:29:PHE:HB2	1:C:296:GLN:NE2	2.06	0.69
1:D:357:LEU:HG	1:D:366:LEU:HD23	1.74	0.69
1:C:369:VAL:HA	1:C:372:GLU:OE2	1.92	0.69
1:C:158:LEU:HD22	1:C:172:LEU:HD21	1.75	0.69
1:A:198:SER:HB3	1:A:218:ASN:HD21	1.57	0.69
1:A:7:TYR:CD2	1:A:211:LYS:HD2	2.28	0.69
1:C:16:MSE:HE1	1:C:249:LEU:HB2	1.75	0.68
1:D:210:LEU:O	1:D:212:ASN:N	2.26	0.68
1:A:165:CYS:HB2	1:A:167:ILE:HD12	1.74	0.68
1:A:196:PRO:O	1:A:225:GLN:NE2	2.27	0.68
1:C:29:PHE:CA	1:C:296:GLN:HG2	2.18	0.68
1:D:29:PHE:HA	1:D:296:GLN:HG2	1.75	0.68
1:D:165:CYS:HB2	1:D:167:ILE:HD12	1.75	0.68
1:B:224:THR:HG22	1:B:228:LEU:HD12	1.74	0.68
1:B:324:VAL:HG12	1:B:324:VAL:O	1.94	0.68
1:C:236:LEU:O	1:C:310:LYS:HE3	1.92	0.68
1:A:274:LEU:HD22	1:A:277:LEU:HD22	1.76	0.67
1:A:454:LYS:NZ	1:A:454:LYS:CD	2.57	0.67
1:B:399:HIS:CE1	1:B:403:ILE:CD1	2.77	0.67
1:C:127:ALA:HB2	1:C:149:GLU:HG3	1.74	0.67
1:A:210:LEU:O	1:A:212:ASN:N	2.28	0.67
1:C:106:LEU:HB3	1:C:107:PRO:HD3	1.76	0.67
1:A:45:THR:HG22	1:A:45:THR:O	1.93	0.67
1:A:445:PHE:HB3	1:A:450:ILE:HD12	1.77	0.67
1:B:242:LEU:HD23	1:B:308:LEU:HD11	1.76	0.67
1:C:172:LEU:HD12	1:C:382:ARG:HB3	1.76	0.67
1:B:102:ALA:HA	1:B:105:MSE:HE3	1.76	0.67
1:C:176:ASP:O	1:C:176:ASP:CG	2.36	0.67
1:D:127:ALA:HB1	1:D:154:ARG:HG2	1.76	0.67
1:B:122:MSE:CE	1:B:146:LEU:HD22	2.25	0.67
1:B:184:VAL:HG12	1:B:187:MSE:CB	2.25	0.67
1:A:197:CYS:HB2	1:A:248:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ASP:HB3	1:A:455:ARG:HE	1.61	0.66
1:C:156:LYS:O	1:C:156:LYS:HE2	1.95	0.66
1:D:96:LEU:HD21	1:D:448:GLN:HG3	1.78	0.66
1:C:328:PRO:O	1:C:360:ARG:HG3	1.96	0.66
1:D:178:ARG:HH11	1:D:178:ARG:CG	2.09	0.65
1:B:176:ASP:O	1:B:176:ASP:OD1	2.14	0.65
1:B:414:PHE:CE2	1:B:436:PRO:HD3	2.30	0.65
1:D:226:ARG:O	1:D:229:ILE:HG22	1.96	0.65
1:A:466:ARG:O	1:A:469:VAL:HG12	1.97	0.65
1:C:230:ASP:OD2	1:C:265:TYR:OH	2.09	0.65
1:D:429:ASP:OD1	1:D:462:ASN:N	2.27	0.65
1:A:287:GLU:HG3	1:B:379:ARG:NE	2.11	0.65
1:B:341:ARG:CG	1:B:351:TRP:CZ2	2.65	0.65
1:C:101:GLU:HB3	1:C:301:GLU:OE2	1.95	0.65
1:D:42:ARG:HE	1:D:100:GLN:HE21	1.44	0.64
1:D:448:GLN:O	1:D:450:ILE:HD13	1.97	0.64
1:D:296:GLN:H	1:D:296:GLN:HE21	1.44	0.64
1:D:122:MSE:HE2	1:D:146:LEU:HD22	1.79	0.64
1:D:150:PHE:HD2	1:D:176:ASP:HA	1.62	0.64
1:A:369:VAL:HA	1:A:372:GLU:OE1	1.97	0.64
1:D:341:ARG:CG	1:D:351:TRP:CZ2	2.79	0.64
1:D:357:LEU:HG	1:D:366:LEU:CD2	2.28	0.63
1:D:37:LEU:HD12	1:D:38:ARG:H	1.63	0.63
1:B:20:MSE:HE1	1:B:296:GLN:OE1	1.99	0.63
1:C:191:ILE:HD12	1:C:236:LEU:HB2	1.80	0.63
1:D:219:GLN:OE1	1:D:219:GLN:HA	1.98	0.63
1:D:150:PHE:CD2	1:D:176:ASP:HA	2.32	0.63
1:B:189:ASP:HB2	1:B:237:ARG:NH1	2.14	0.62
1:D:7:TYR:HE2	1:D:211:LYS:HA	1.63	0.62
1:D:351:TRP:CE3	1:D:352:ASP:O	2.51	0.62
1:A:153:SER:O	1:A:156:LYS:HD3	2.00	0.62
1:A:210:LEU:HD12	1:A:211:LYS:N	2.14	0.62
1:D:58:ALA:N	1:D:59:PRO:HD2	2.14	0.62
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.82	0.62
1:B:122:MSE:HE3	1:B:146:LEU:HD22	1.82	0.62
1:D:7:TYR:CE2	1:D:211:LYS:HA	2.35	0.62
1:C:221:ILE:O	1:C:225:GLN:HG3	2.00	0.61
1:C:226:ARG:O	1:C:229:ILE:HG22	2.00	0.61
1:B:351:TRP:O	1:B:351:TRP:CE3	2.52	0.61
1:A:430:VAL:O	1:A:459:ARG:O	2.18	0.61
1:D:274:LEU:HD22	1:D:277:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLY:HA2	1:B:341:ARG:HD2	1.83	0.61
1:C:142:GLU:HA	1:C:142:GLU:OE2	2.01	0.61
1:A:396:ARG:O	1:A:398:GLN:NE2	2.33	0.60
1:B:324:VAL:O	1:B:324:VAL:CG1	2.49	0.60
1:B:108:VAL:HG13	1:B:135:ILE:HD13	1.84	0.60
1:B:341:ARG:HB3	1:B:351:TRP:CZ2	2.37	0.60
1:B:225:GLN:NE2	1:B:253:GLU:HB3	2.10	0.60
1:A:445:PHE:HB3	1:A:450:ILE:HD11	1.83	0.60
1:C:108:VAL:CG1	1:C:134:GLN:HG2	2.29	0.60
1:C:236:LEU:HD11	1:C:240:GLY:CA	2.30	0.60
1:A:223:ALA:CA	1:A:226:ARG:NH1	2.61	0.59
1:A:29:PHE:CA	1:A:296:GLN:HG2	2.33	0.59
1:A:58:ALA:N	1:A:59:PRO:HD2	2.16	0.59
1:B:162:ILE:CD1	1:B:170:VAL:HG11	2.33	0.59
1:D:127:ALA:H	1:D:149:GLU:HG2	1.66	0.59
1:C:94:SER:HB3	1:C:450:ILE:HD11	1.85	0.59
1:A:318:PRO:O	1:A:320:PRO:CD	2.43	0.59
1:B:42:ARG:HE	1:B:100:GLN:NE2	2.00	0.59
1:D:26:PHE:O	1:D:29:PHE:HB3	2.01	0.59
1:C:16:MSE:HE1	1:C:249:LEU:CB	2.33	0.59
1:C:456:ILE:HG21	1:C:459:ARG:NH2	2.18	0.58
1:A:202:VAL:HG12	1:A:202:VAL:O	2.03	0.58
1:D:103:SER:HB2	1:D:301:GLU:CD	2.27	0.58
1:D:410:ASN:HD22	1:D:413:ALA:N	2.01	0.58
1:B:42:ARG:HE	1:B:100:GLN:HE21	1.51	0.58
1:B:40:SER:OG	1:B:100:GLN:O	2.20	0.58
1:C:229:ILE:HG12	1:C:261:LEU:HD22	1.86	0.58
1:D:178:ARG:HG3	1:D:178:ARG:NH1	2.17	0.58
1:D:192:LEU:HD23	1:D:192:LEU:C	2.28	0.58
1:C:456:ILE:HG21	1:C:459:ARG:HH22	1.69	0.58
1:D:286:THR:HG1	1:D:290:PHE:HB2	1.69	0.58
1:B:162:ILE:HG23	1:B:167:ILE:HB	1.86	0.58
1:C:338:GLY:HA2	1:C:341:ARG:HH21	1.68	0.58
1:A:445:PHE:CB	1:A:450:ILE:HD12	2.33	0.58
1:D:200:GLU:CD	1:D:249:LEU:H	2.11	0.57
1:D:430:VAL:O	1:D:459:ARG:O	2.22	0.57
1:C:278:PHE:HB2	1:C:279:PRO:HD2	1.86	0.57
1:B:146:LEU:HD23	1:B:146:LEU:C	2.30	0.57
1:C:16:MSE:HE3	1:C:29:PHE:CZ	2.39	0.57
1:A:7:TYR:O	1:A:210:LEU:HD11	2.04	0.57
1:A:45:THR:HA	1:A:48:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:SER:OG	1:A:131:LYS:HE3	2.05	0.57
1:B:337:ALA:O	1:B:341:ARG:HG3	2.05	0.57
1:B:27:ASP:OD2	1:B:27:ASP:N	2.29	0.57
1:D:221:ILE:O	1:D:224:THR:HB	2.05	0.57
1:B:29:PHE:CA	1:B:296:GLN:HG2	2.29	0.57
1:C:398:GLN:O	1:C:402:VAL:HG23	2.05	0.57
1:A:69:TRP:CG	1:A:106:LEU:HD13	2.40	0.56
1:B:201:GLY:O	1:B:301:GLU:HG2	2.05	0.56
1:D:286:THR:OG1	1:D:290:PHE:HB2	2.04	0.56
1:A:357:LEU:HD13	1:A:366:LEU:HD21	1.88	0.56
1:B:136:SER:HB3	1:B:167:ILE:HD12	1.87	0.56
1:C:129:GLY:O	1:C:133:THR:HG23	2.05	0.56
1:B:352:ASP:CB	1:B:354:ASN:H	2.18	0.56
1:C:29:PHE:HB2	1:C:296:GLN:HE21	1.70	0.56
1:A:197:CYS:HB2	1:A:248:THR:HG22	1.88	0.56
1:B:350:ASN:O	1:B:405:LEU:HB3	2.05	0.56
1:A:141:ASN:HD21	1:A:168:SER:H	1.53	0.56
1:C:47:LYS:NZ	1:C:403:ILE:HG23	2.20	0.56
1:C:322:TYR:O	1:C:323:LYS:C	2.49	0.56
1:B:46:LEU:CD1	1:B:167:ILE:HD13	2.35	0.55
1:D:250:ASN:ND2	1:D:253:GLU:H	2.04	0.55
1:B:185:PRO:O	1:B:235:ALA:HA	2.06	0.55
1:B:216:GLU:OE2	1:B:216:GLU:N	2.38	0.55
1:B:349:LEU:HD21	1:B:402:VAL:HA	1.86	0.55
1:D:250:ASN:HD21	1:D:253:GLU:H	1.53	0.55
1:C:470:ARG:HG2	1:C:474:LEU:HD21	1.88	0.55
1:B:272:LEU:HB3	1:B:307:ARG:HE	1.71	0.55
1:C:105:MSE:HA	1:C:134:GLN:HE22	1.72	0.55
1:B:430:VAL:O	1:B:459:ARG:O	2.24	0.55
1:D:37:LEU:HD21	1:D:301:GLU:OE1	2.07	0.55
1:C:242:LEU:HD12	1:C:243:VAL:N	2.22	0.55
1:D:132:THR:HG21	1:D:147:ALA:HB2	1.87	0.55
1:B:106:LEU:HB3	1:B:107:PRO:HD3	1.87	0.55
1:D:26:PHE:C	1:D:26:PHE:CD2	2.84	0.55
1:C:47:LYS:HZ1	1:C:403:ILE:HG23	1.70	0.55
1:A:261:LEU:HD23	1:A:308:LEU:CD2	2.37	0.54
1:D:37:LEU:HD21	1:D:301:GLU:HG3	1.87	0.54
1:D:222:ALA:O	1:D:226:ARG:HG2	2.07	0.54
1:D:352:ASP:HB3	1:D:354:ASN:H	1.72	0.54
1:B:415:GLU:OE1	1:B:446:GLN:N	2.41	0.54
1:A:415:GLU:OE2	1:A:446:GLN:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:GLU:HB3	1:D:237:ARG:HA	1.89	0.54
1:C:445:PHE:C	1:C:446:GLN:HG2	2.33	0.54
1:D:272:LEU:HD11	1:D:309:ARG:HB2	1.88	0.54
1:A:270:GLU:OE2	1:A:309:ARG:NH2	2.41	0.54
1:D:127:ALA:HB2	1:D:149:GLU:CG	2.36	0.54
1:B:237:ARG:HH21	1:B:239:GLY:HA3	1.73	0.54
1:D:347:VAL:HG12	1:D:347:VAL:O	2.07	0.54
1:D:332:VAL:HG13	1:D:336:GLU:OE2	2.07	0.54
1:D:206:ASP:HB3	1:D:209:ALA:HB2	1.89	0.54
1:A:252:GLU:CD	1:A:252:GLU:H	2.15	0.53
1:B:162:ILE:HD13	1:B:170:VAL:HG11	1.89	0.53
1:B:186:GLU:HB3	1:B:237:ARG:HA	1.89	0.53
1:B:215:PRO:O	1:B:218:ASN:HB2	2.09	0.53
1:D:202:VAL:HG12	1:D:202:VAL:O	2.08	0.53
1:A:406:ALA:HB3	1:A:449:PRO:HB3	1.91	0.53
1:B:113:ALA:HB3	1:B:307:ARG:NH1	2.22	0.53
1:D:410:ASN:ND2	1:D:412:ASN:OD1	2.41	0.53
1:A:129:GLY:O	1:A:133:THR:HG23	2.08	0.53
1:D:233:PHE:CZ	1:D:310:LYS:HG3	2.43	0.53
1:A:330:SER:OG	1:A:331:PRO:HD2	2.08	0.53
1:C:8:PHE:CD1	1:C:8:PHE:N	2.74	0.53
1:C:218:ASN:ND2	1:C:253:GLU:OE2	2.41	0.53
1:A:12:PHE:CE2	1:A:13:LEU:HD23	2.44	0.53
1:D:415:GLU:HG2	1:D:444:THR:OG1	2.08	0.53
1:D:416:LEU:HD13	1:D:421:ALA:HA	1.90	0.53
1:B:347:VAL:CG1	1:B:347:VAL:O	2.57	0.53
1:C:335:ARG:NH1	1:C:336:GLU:H	2.07	0.53
1:C:430:VAL:O	1:C:459:ARG:O	2.27	0.53
1:B:341:ARG:CB	1:B:351:TRP:CZ2	2.92	0.52
1:A:424:TRP:HH2	1:A:453:ALA:HB2	1.74	0.52
1:C:29:PHE:HA	1:C:296:GLN:CG	2.20	0.52
1:C:466:ARG:C	1:C:468:LEU:H	2.18	0.52
1:D:158:LEU:O	1:D:162:ILE:HG13	2.10	0.52
1:D:162:ILE:HG23	1:D:167:ILE:HB	1.90	0.52
1:D:229:ILE:HD13	1:D:244:TYR:CD2	2.44	0.52
1:B:226:ARG:HD2	1:B:260:TRP:CD2	2.45	0.52
1:A:26:PHE:C	1:A:26:PHE:CD2	2.87	0.52
1:D:29:PHE:CA	1:D:296:GLN:HG2	2.40	0.52
1:D:197:CYS:HB2	1:D:253:GLU:OE2	2.09	0.52
1:D:466:ARG:HA	1:D:469:VAL:HG13	1.91	0.52
1:B:356:ARG:HH11	1:B:356:ARG:HG2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:GLU:HG3	1:D:248:THR:HA	1.91	0.52
1:A:417:THR:HB	1:A:418:PRO:HD2	1.92	0.52
1:D:208:ASP:O	1:D:211:LYS:HG3	2.09	0.52
1:B:17:ARG:NH2	1:B:26:PHE:CE2	2.76	0.52
1:C:165:CYS:HB2	1:C:167:ILE:HD12	1.92	0.52
1:D:180:PHE:O	1:D:184:VAL:HG12	2.10	0.52
1:A:269:VAL:CG1	1:A:308:LEU:HD23	2.39	0.51
1:A:127:ALA:HB3	1:A:149:GLU:OE2	2.10	0.51
1:A:186:GLU:HB3	1:A:237:ARG:HA	1.92	0.51
1:D:29:PHE:HA	1:D:296:GLN:HG3	1.90	0.51
1:D:445:PHE:C	1:D:446:GLN:HG2	2.35	0.51
1:A:210:LEU:HD12	1:A:211:LYS:H	1.76	0.51
1:A:261:LEU:HD23	1:A:308:LEU:HD22	1.91	0.51
1:B:202:VAL:HG12	1:B:202:VAL:O	2.10	0.51
1:C:35:ARG:HH21	1:C:299:ASP:CG	2.19	0.51
1:D:368:PRO:O	1:D:371:ILE:HG22	2.11	0.51
1:D:341:ARG:HG3	1:D:351:TRP:HZ2	1.75	0.51
1:A:439:ASP:HA	1:A:455:ARG:HB2	1.92	0.51
1:C:193:LEU:HD23	1:C:244:TYR:CD2	2.46	0.51
1:C:245:SER:HA	1:C:304:PHE:O	2.11	0.51
1:B:425:TYR:OH	1:B:450:ILE:HD11	2.07	0.50
1:B:473:LYS:C	1:B:474:LEU:HG	2.36	0.50
1:D:420:GLU:OE1	1:D:420:GLU:CG	2.55	0.50
1:A:184:VAL:HG22	1:A:187:MSE:HB2	1.92	0.50
1:C:102:ALA:HA	1:C:105:MSE:HE3	1.92	0.50
1:D:184:VAL:HG22	1:D:187:MSE:HB2	1.92	0.50
1:D:324:VAL:HG12	1:D:379:ARG:NE	2.21	0.50
1:B:122:MSE:HE1	1:B:180:PHE:CD2	2.42	0.50
1:C:127:ALA:H	1:C:149:GLU:HG2	1.77	0.50
1:D:265:TYR:HB3	1:D:268:ALA:HB3	1.93	0.50
1:D:338:GLY:O	1:D:341:ARG:HB2	2.11	0.50
1:D:466:ARG:C	1:D:468:LEU:H	2.20	0.50
1:C:341:ARG:CB	1:C:351:TRP:CZ2	2.92	0.50
1:A:187:MSE:CE	1:A:187:MSE:HB2	2.42	0.50
1:A:273:PRO:HA	1:A:289:GLY:HA3	1.94	0.50
1:D:37:LEU:HD12	1:D:38:ARG:N	2.27	0.50
1:A:426:ARG:NH2	1:A:472:GLY:O	2.44	0.49
1:C:111:LEU:HD12	1:C:243:VAL:HG23	1.93	0.49
1:D:406:ALA:HB3	1:D:449:PRO:HB3	1.94	0.49
1:B:224:THR:HG22	1:B:228:LEU:CD1	2.40	0.49
1:D:250:ASN:HD22	1:D:252:GLU:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:VAL:HA	1:D:379:ARG:HH21	1.76	0.49
1:A:29:PHE:O	1:A:33:CYS:HB2	2.13	0.49
1:C:20:MSE:HE1	1:C:294:PHE:CD1	2.48	0.49
1:C:101:GLU:CB	1:C:301:GLU:OE2	2.59	0.49
1:A:252:GLU:OE2	1:A:252:GLU:N	2.39	0.49
1:A:470:ARG:HG2	1:A:474:LEU:HD21	1.94	0.49
1:B:294:PHE:HB3	1:B:295:PRO:HD2	1.95	0.49
1:C:193:LEU:HD23	1:C:244:TYR:HD2	1.77	0.49
1:C:288:GLU:N	1:C:288:GLU:OE1	2.45	0.49
1:C:446:GLN:O	1:C:447:HIS:HB2	2.12	0.49
1:D:234:HIS:CE1	1:D:314:ILE:CD1	2.95	0.49
1:A:286:THR:HB	1:A:288:GLU:OE2	2.13	0.49
1:B:186:GLU:O	1:B:237:ARG:HB3	2.11	0.49
1:D:456:ILE:HG21	1:D:459:ARG:HE	1.77	0.49
1:A:414:PHE:CE2	1:A:436:PRO:HD3	2.48	0.49
1:C:184:VAL:HG13	1:C:184:VAL:O	2.13	0.49
1:D:146:LEU:HD23	1:D:146:LEU:C	2.37	0.49
1:A:424:TRP:CH2	1:A:453:ALA:HB2	2.47	0.49
1:C:309:ARG:HG3	1:C:309:ARG:HH11	1.78	0.49
1:A:347:VAL:O	1:A:347:VAL:CG1	2.61	0.48
1:B:40:SER:OG	1:B:101:GLU:HA	2.11	0.48
1:B:335:ARG:CG	1:B:335:ARG:NH1	2.42	0.48
1:C:226:ARG:HD3	1:C:260:TRP:CG	2.48	0.48
1:D:45:THR:O	1:D:45:THR:HG22	2.13	0.48
1:A:120:ARG:HH11	1:A:120:ARG:HG2	1.77	0.48
1:A:322:TYR:O	1:A:323:LYS:C	2.56	0.48
1:B:146:LEU:HD21	1:B:173:THR:OG1	2.13	0.48
1:C:419:GLN:OE1	1:C:419:GLN:HA	2.13	0.48
1:D:103:SER:OG	1:D:303:PHE:CE1	2.61	0.48
1:A:182:ALA:HB1	1:A:319:ALA:HB3	1.95	0.48
1:C:431:TYR:N	1:C:431:TYR:CD1	2.81	0.48
1:C:445:PHE:O	1:C:446:GLN:HG2	2.13	0.48
1:A:221:ILE:O	1:A:225:GLN:CG	2.60	0.48
1:A:473:LYS:H	1:A:473:LYS:HZ3	1.61	0.48
1:D:420:GLU:OE1	1:D:420:GLU:CB	2.61	0.48
1:A:424:TRP:NE1	1:A:464:TYR:HB2	2.29	0.48
1:B:399:HIS:NE2	1:B:403:ILE:HD11	2.26	0.48
1:D:406:ALA:HB1	1:D:442:LEU:HD21	1.95	0.48
1:D:471:ASP:OD2	1:D:471:ASP:N	2.43	0.48
1:B:286:THR:HG23	1:B:290:PHE:O	2.13	0.48
1:D:290:PHE:CD2	1:D:304:PHE:HZ	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:LEU:HD21	1:D:301:GLU:CG	2.44	0.48
1:C:90:ALA:HA	1:C:93:LEU:HD12	1.95	0.48
1:B:122:MSE:CE	1:B:180:PHE:CZ	2.97	0.48
1:C:108:VAL:CG2	1:C:134:GLN:HE21	2.27	0.48
1:C:127:ALA:HB2	1:C:149:GLU:CG	2.40	0.48
1:B:13:LEU:C	1:B:15:GLN:H	2.22	0.47
1:C:108:VAL:HG21	1:C:134:GLN:HE21	1.79	0.47
1:A:296:GLN:H	1:A:296:GLN:HG3	1.39	0.47
1:D:317:LEU:HB3	1:D:318:PRO:HD2	1.96	0.47
1:A:41:ILE:HG13	1:A:97:PHE:CD1	2.49	0.47
1:A:223:ALA:HA	1:A:226:ARG:HH12	1.72	0.47
1:B:199:GLY:O	1:B:202:VAL:HB	2.14	0.47
1:A:180:PHE:O	1:A:184:VAL:HG12	2.14	0.47
1:D:37:LEU:CD2	1:D:301:GLU:HG3	2.45	0.47
1:B:108:VAL:CG1	1:B:134:GLN:HG2	2.43	0.47
1:B:234:HIS:CE1	1:B:314:ILE:HD13	2.50	0.47
1:B:432:PRO:HG2	1:B:435:ALA:HA	1.97	0.47
1:D:273:PRO:HA	1:D:289:GLY:HA3	1.97	0.47
1:A:42:ARG:NH2	1:A:134:GLN:HA	2.29	0.47
1:C:341:ARG:HD3	1:C:351:TRP:CZ2	2.47	0.47
1:D:260:TRP:O	1:D:263:GLU:HB2	2.15	0.47
1:A:45:THR:O	1:A:45:THR:CG2	2.60	0.47
1:C:32:ALA:HB2	1:C:296:GLN:HB3	1.97	0.47
1:C:32:ALA:CB	1:C:296:GLN:HB3	2.45	0.47
1:D:322:TYR:O	1:D:323:LYS:C	2.57	0.47
1:A:198:SER:CB	1:A:218:ASN:HD21	2.26	0.47
1:B:136:SER:CB	1:B:167:ILE:HD12	2.45	0.47
1:B:184:VAL:O	1:B:185:PRO:O	2.32	0.47
1:B:296:GLN:HE21	1:B:296:GLN:HB2	1.53	0.47
1:C:410:ASN:OD1	1:C:412:ASN:N	2.48	0.47
1:D:234:HIS:HE1	1:D:265:TYR:OH	1.98	0.47
1:C:37:LEU:HG	1:C:204:ARG:HB2	1.98	0.46
1:D:91:GLU:CD	1:D:91:GLU:H	2.22	0.46
1:D:210:LEU:HB2	1:D:213:TRP:HB2	1.96	0.46
1:D:347:VAL:HG11	1:D:452:LEU:HD11	1.97	0.46
1:D:426:ARG:HH11	1:D:474:LEU:HD12	1.79	0.46
1:C:187:MSE:CE	1:C:187:MSE:HB2	2.45	0.46
1:C:336:GLU:HA	1:C:339:GLN:HG2	1.96	0.46
1:D:459:ARG:O	1:D:460:LEU:HB2	2.15	0.46
1:B:358:TRP:CD1	1:B:367:PHE:CD2	3.03	0.46
1:C:13:LEU:C	1:C:15:GLN:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ARG:HG3	1:C:238:PRO:O	2.16	0.46
1:C:106:LEU:HB3	1:C:107:PRO:CD	2.44	0.46
1:C:111:LEU:HD23	1:C:112:PHE:CE2	2.51	0.46
1:C:366:LEU:O	1:C:384:GLY:HA3	2.16	0.46
1:C:466:ARG:C	1:C:468:LEU:N	2.74	0.46
1:D:29:PHE:O	1:D:33:CYS:HB2	2.15	0.46
1:A:184:VAL:HG22	1:A:187:MSE:CB	2.46	0.46
1:A:246:THR:OG1	1:A:254:ASN:OD1	2.29	0.46
1:D:424:TRP:NE1	1:D:464:TYR:HB2	2.30	0.46
1:C:351:TRP:HE3	1:C:351:TRP:O	1.98	0.46
1:A:169:ASN:C	1:A:169:ASN:HD22	2.22	0.46
1:D:122:MSE:HE3	1:D:146:LEU:HD22	1.95	0.46
1:D:167:ILE:HG21	1:D:170:VAL:HG23	1.98	0.46
1:D:338:GLY:HA2	1:D:341:ARG:HD2	1.97	0.46
1:B:55:GLN:HE21	1:B:55:GLN:HB3	1.57	0.46
1:C:362:LYS:H	1:C:362:LYS:HG2	1.43	0.46
1:D:101:GLU:H	1:D:101:GLU:HG2	1.33	0.46
1:D:357:LEU:HD12	1:D:357:LEU:N	2.31	0.46
1:D:42:ARG:HE	1:D:100:GLN:NE2	2.12	0.45
1:A:146:LEU:HD11	1:A:173:THR:HG21	1.98	0.45
1:B:131:LYS:O	1:B:134:GLN:HB3	2.17	0.45
1:C:216:GLU:OE2	1:C:216:GLU:HA	2.16	0.45
1:C:226:ARG:HG2	1:C:260:TRP:CE3	2.51	0.45
1:D:200:GLU:HG2	1:D:248:THR:OG1	2.16	0.45
1:D:464:TYR:HE2	1:D:469:VAL:HA	1.81	0.45
1:A:427:GLY:HA2	1:A:462:ASN:ND2	2.31	0.45
1:A:35:ARG:HG3	1:A:204:ARG:HH21	1.81	0.45
1:A:197:CYS:CB	1:A:248:THR:HG22	2.46	0.45
1:B:321:LYS:HD2	1:B:321:LYS:HA	1.77	0.45
1:B:341:ARG:CB	1:B:351:TRP:HZ2	2.24	0.45
1:C:432:PRO:HG2	1:C:435:ALA:HA	1.98	0.45
1:D:103:SER:OG	1:D:303:PHE:CD1	2.65	0.45
1:A:362:LYS:O	1:A:390:THR:OG1	2.33	0.45
1:B:455:ARG:O	1:B:456:ILE:C	2.59	0.45
1:B:466:ARG:C	1:B:468:LEU:H	2.24	0.45
1:C:199:GLY:O	1:C:202:VAL:HB	2.16	0.45
1:C:273:PRO:HA	1:C:289:GLY:HA3	1.99	0.45
1:B:246:THR:OG1	1:B:254:ASN:ND2	2.37	0.45
1:C:44:ASN:OD1	1:C:44:ASN:C	2.60	0.45
1:D:432:PRO:HG2	1:D:435:ALA:HA	1.98	0.45
1:D:300:CYS:HB2	1:D:301:GLU:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:PHE:CE1	1:D:383:LEU:HB2	2.51	0.45
1:D:420:GLU:HG2	1:D:430:VAL:HG13	1.98	0.45
1:C:142:GLU:OE2	1:C:142:GLU:CA	2.65	0.45
1:D:8:PHE:HE1	1:D:34:GLN:HE22	1.65	0.45
1:D:347:VAL:CG1	1:D:452:LEU:HD11	2.47	0.44
1:A:233:PHE:CZ	1:A:269:VAL:HG22	2.52	0.44
1:A:329:PHE:CZ	1:A:360:ARG:NH1	2.86	0.44
1:B:226:ARG:HD2	1:B:260:TRP:CE2	2.52	0.44
1:C:65:THR:HB	1:C:75:TRP:HB2	1.99	0.44
1:A:466:ARG:C	1:A:468:LEU:H	2.26	0.44
1:B:336:GLU:O	1:B:337:ALA:C	2.61	0.44
1:D:97:PHE:C	1:D:97:PHE:CD1	2.96	0.44
1:B:184:VAL:HG12	1:B:184:VAL:O	2.17	0.44
1:B:131:LYS:NZ	1:B:194:ASP:OD1	2.29	0.44
1:C:341:ARG:HH11	1:C:351:TRP:HH2	1.65	0.44
1:C:367:PHE:CD1	1:C:383:LEU:HB2	2.52	0.44
1:A:20:MSE:HA	1:A:21:PRO:HD3	1.79	0.44
1:A:423:GLU:HG3	1:A:428:ARG:HB2	2.00	0.44
1:B:56:LEU:HD11	1:B:446:GLN:HG2	2.00	0.44
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.65	0.44
1:C:259:LEU:HA	1:C:259:LEU:HD23	1.71	0.44
1:C:296:GLN:H	1:C:296:GLN:HG3	1.39	0.44
1:D:454:LYS:HB3	1:D:454:LYS:HE2	1.78	0.44
1:B:386:LYS:HD2	1:B:398:GLN:HG3	2.00	0.44
1:B:456:ILE:HD12	1:B:459:ARG:HD2	1.99	0.44
1:C:202:VAL:O	1:C:202:VAL:CG1	2.65	0.44
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.73	0.44
1:A:149:GLU:HA	1:A:149:GLU:OE1	2.18	0.44
1:B:462:ASN:ND2	1:B:464:TYR:H	2.16	0.44
1:B:466:ARG:C	1:B:468:LEU:N	2.75	0.44
1:C:415:GLU:OE1	1:C:445:PHE:HA	2.18	0.44
1:A:7:TYR:C	1:A:8:PHE:CD2	2.96	0.43
1:C:88:SER:HB3	1:C:470:ARG:HE	1.82	0.43
1:C:456:ILE:CG2	1:C:459:ARG:NH2	2.81	0.43
1:D:40:SER:OG	1:D:101:GLU:HA	2.17	0.43
1:B:39:ARG:H	1:B:39:ARG:HG3	1.55	0.43
1:B:86:LEU:CD2	1:B:97:PHE:CZ	3.01	0.43
1:C:336:GLU:O	1:C:337:ALA:C	2.61	0.43
1:C:446:GLN:HE21	1:C:446:GLN:HB3	1.64	0.43
1:C:86:LEU:O	1:C:89:THR:HG22	2.18	0.43
1:C:186:GLU:HB2	1:C:237:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:O	1:A:347:VAL:HG12	2.17	0.43
1:B:386:LYS:HB3	1:B:398:GLN:HG3	1.99	0.43
1:C:374:LEU:HD12	1:C:374:LEU:N	2.33	0.43
1:D:466:ARG:C	1:D:468:LEU:N	2.73	0.43
1:B:112:PHE:N	1:B:112:PHE:CD2	2.86	0.43
1:B:356:ARG:HG2	1:B:356:ARG:NH1	2.34	0.43
1:D:135:ILE:O	1:D:139:MSE:HG3	2.19	0.43
1:A:169:ASN:HD22	1:A:170:VAL:HG23	1.84	0.43
1:B:357:LEU:HD12	1:B:357:LEU:H	1.84	0.43
1:B:410:ASN:ND2	1:B:412:ASN:OD1	2.52	0.43
1:C:120:ARG:NE	1:C:370:GLY:O	2.52	0.43
1:C:236:LEU:O	1:C:310:LYS:CE	2.65	0.43
1:D:225:GLN:HE22	1:D:253:GLU:CG	2.27	0.43
1:A:174:HIS:ND1	1:A:174:HIS:O	2.47	0.43
1:B:12:PHE:HE1	1:B:200:GLU:OE1	2.01	0.43
1:B:91:GLU:HG3	1:B:96:LEU:HD12	1.99	0.43
1:C:351:TRP:O	1:C:351:TRP:CE3	2.72	0.43
1:A:328:PRO:HG2	1:A:329:PHE:CE1	2.53	0.43
1:B:294:PHE:H	1:B:297:ILE:CD1	2.31	0.43
1:D:415:GLU:OE1	1:D:445:PHE:HA	2.19	0.43
1:A:13:LEU:C	1:A:15:GLN:H	2.26	0.43
1:C:69:TRP:CG	1:C:106:LEU:HD13	2.53	0.43
1:D:357:LEU:HD12	1:D:357:LEU:H	1.83	0.43
1:A:318:PRO:HB2	1:A:319:ALA:HA	2.00	0.43
1:C:9:PRO:HD3	1:C:210:LEU:HD13	2.01	0.43
1:C:335:ARG:HB3	1:C:335:ARG:NH1	2.06	0.43
1:D:120:ARG:HH11	1:D:187:MSE:HG3	1.84	0.43
1:D:427:GLY:HA2	1:D:462:ASN:OD1	2.19	0.43
1:B:294:PHE:H	1:B:297:ILE:HD12	1.83	0.42
1:C:424:TRP:HH2	1:C:453:ALA:HB2	1.84	0.42
1:D:272:LEU:CB	1:D:307:ARG:HE	2.32	0.42
1:B:296:GLN:H	1:B:296:GLN:HG3	1.34	0.42
1:C:366:LEU:HD11	1:C:387:LEU:HD22	2.02	0.42
1:C:466:ARG:O	1:C:469:VAL:HG22	2.20	0.42
1:B:112:PHE:HZ	1:B:135:ILE:HG23	1.84	0.42
1:C:158:LEU:HD23	1:C:162:ILE:HD12	2.00	0.42
1:D:214:SER:HB3	1:D:217:SER:HB3	2.00	0.42
1:D:371:ILE:HD12	1:D:374:LEU:CD1	2.49	0.42
1:D:409:ASP:OD1	1:D:409:ASP:N	2.53	0.42
1:C:417:THR:HB	1:C:418:PRO:HD2	2.01	0.42
1:C:424:TRP:CH2	1:C:453:ALA:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LEU:HB2	1:D:307:ARG:HE	1.84	0.42
1:A:37:LEU:HD11	1:A:301:GLU:HG3	2.00	0.42
1:A:225:GLN:OE1	1:A:253:GLU:CG	2.55	0.42
1:A:466:ARG:C	1:A:468:LEU:N	2.77	0.42
1:B:44:ASN:OD1	1:B:44:ASN:C	2.63	0.42
1:C:420:GLU:HG2	1:C:430:VAL:HG13	2.02	0.42
1:D:187:MSE:HB3	1:D:188:PHE:CD2	2.54	0.42
1:D:225:GLN:NE2	1:D:253:GLU:HG2	2.30	0.42
1:D:334:ASP:O	1:D:335:ARG:C	2.61	0.42
1:B:347:VAL:O	1:B:347:VAL:HG12	2.18	0.42
1:B:86:LEU:CD2	1:B:97:PHE:CE1	3.02	0.42
1:B:210:LEU:HB2	1:B:213:TRP:HB2	2.02	0.42
1:C:233:PHE:CZ	1:C:310:LYS:HG3	2.54	0.42
1:D:250:ASN:ND2	1:D:250:ASN:C	2.78	0.42
1:C:20:MSE:HG2	1:C:26:PHE:HA	2.01	0.42
1:C:96:LEU:HD21	1:C:448:GLN:HG3	2.01	0.42
1:C:416:LEU:HD22	1:C:420:GLU:HB3	2.02	0.42
1:A:319:ALA:N	1:A:320:PRO:HD3	2.30	0.42
1:B:62:TRP:HE3	1:B:64:LEU:HD11	1.84	0.42
1:C:406:ALA:HB3	1:C:449:PRO:HB3	2.00	0.42
1:D:296:GLN:HE21	1:D:296:GLN:N	2.14	0.42
1:A:34:GLN:HE21	1:A:34:GLN:HB2	1.72	0.41
1:A:226:ARG:HG3	1:A:260:TRP:CE3	2.55	0.41
1:B:467:GLU:H	1:B:467:GLU:CD	2.28	0.41
1:C:206:ASP:HB3	1:C:209:ALA:HB2	2.02	0.41
1:C:327:PHE:CD2	1:C:328:PRO:HD2	2.55	0.41
1:D:195:ALA:HA	1:D:196:PRO:HD3	1.95	0.41
1:D:340:ILE:HD13	1:D:364:LEU:HD13	2.02	0.41
1:A:101:GLU:H	1:A:101:GLU:HG2	1.63	0.41
1:B:322:TYR:O	1:B:323:LYS:C	2.63	0.41
1:B:385:ILE:HD11	1:B:405:LEU:HD21	2.03	0.41
1:C:334:ASP:O	1:C:335:ARG:C	2.63	0.41
1:D:309:ARG:HH11	1:D:309:ARG:HB3	1.85	0.41
1:A:416:LEU:HD13	1:A:421:ALA:HA	2.02	0.41
1:A:426:ARG:C	1:A:469:VAL:HG23	2.45	0.41
1:A:454:LYS:NZ	1:A:454:LYS:HD2	2.36	0.41
1:B:111:LEU:HD12	1:B:111:LEU:HA	1.85	0.41
1:C:129:GLY:O	1:C:130:SER:C	2.63	0.41
1:C:184:VAL:HG22	1:C:187:MSE:HB2	2.01	0.41
1:D:29:PHE:CD1	1:D:295:PRO:HD2	2.55	0.41
1:A:222:ALA:HA	1:A:225:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ALA:O	1:A:435:ALA:HB3	2.20	0.41
1:A:210:LEU:H	1:A:210:LEU:HG	1.63	0.41
1:B:422:GLU:HB3	1:B:426:ARG:NH2	2.36	0.41
1:C:210:LEU:HB2	1:C:213:TRP:HB2	2.03	0.41
1:D:13:LEU:C	1:D:15:GLN:H	2.29	0.41
1:D:420:GLU:OE1	1:D:420:GLU:HB2	2.21	0.41
1:B:65:THR:HA	1:B:66:PRO:HD3	1.91	0.41
1:C:321:LYS:HD2	1:C:321:LYS:HA	1.65	0.41
1:C:422:GLU:HG3	1:C:474:LEU:HD12	2.02	0.41
1:C:455:ARG:O	1:C:456:ILE:C	2.63	0.41
1:A:146:LEU:HD11	1:A:173:THR:CG2	2.51	0.41
1:A:184:VAL:O	1:A:185:PRO:O	2.39	0.41
1:A:287:GLU:HG3	1:B:379:ARG:CD	2.51	0.41
1:B:250:ASN:O	1:B:254:ASN:OD1	2.39	0.41
1:C:158:LEU:HD23	1:C:162:ILE:CD1	2.51	0.41
1:D:12:PHE:HE1	1:D:200:GLU:OE1	2.04	0.41
1:A:336:GLU:HA	1:A:339:GLN:HG2	2.03	0.41
1:C:162:ILE:HG23	1:C:167:ILE:HB	2.03	0.41
1:C:179:VAL:HG12	1:C:183:ALA:HB2	2.03	0.41
1:D:318:PRO:O	1:D:320:PRO:CG	2.68	0.41
1:A:174:HIS:ND1	1:A:174:HIS:C	2.78	0.40
1:B:250:ASN:OD1	1:B:250:ASN:C	2.64	0.40
1:B:409:ASP:OD1	1:B:409:ASP:N	2.55	0.40
1:D:122:MSE:HE1	1:D:180:PHE:CE2	2.55	0.40
1:A:162:ILE:HG23	1:A:167:ILE:HB	2.03	0.40
1:A:167:ILE:CG2	1:A:170:VAL:HG23	2.52	0.40
1:B:135:ILE:HG12	1:B:135:ILE:H	1.71	0.40
1:B:251:GLN:NE2	1:B:255:GLU:HB2	2.36	0.40
1:C:67:ILE:HA	1:C:68:PRO:HD3	1.97	0.40
1:C:184:VAL:N	1:C:185:PRO:CD	2.83	0.40
1:D:341:ARG:NE	1:D:351:TRP:CH2	2.86	0.40
1:B:146:LEU:C	1:B:146:LEU:CD2	2.94	0.40
1:D:146:LEU:HD21	1:D:173:THR:OG1	2.22	0.40
1:B:245:SER:HA	1:B:304:PHE:O	2.21	0.40
1:B:423:GLU:O	1:B:424:TRP:C	2.63	0.40
1:A:371:ILE:O	1:A:372:GLU:C	2.63	0.40
1:C:41:ILE:HG21	1:C:41:ILE:HD13	1.77	0.40
1:C:415:GLU:OE1	1:C:446:GLN:N	2.54	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	449/479 (94%)	408 (91%)	28 (6%)	13 (3%)	3	15
1	B	448/479 (94%)	401 (90%)	35 (8%)	12 (3%)	4	16
1	C	448/479 (94%)	401 (90%)	33 (7%)	14 (3%)	3	14
1	D	449/479 (94%)	403 (90%)	32 (7%)	14 (3%)	3	14
All	All	1794/1916 (94%)	1613 (90%)	128 (7%)	53 (3%)	3	14

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	PRO
1	A	211	LYS
1	A	409	ASP
1	B	185	PRO
1	B	211	LYS
1	B	319	ALA
1	C	185	PRO
1	C	211	LYS
1	C	319	ALA
1	C	456	ILE
1	D	185	PRO
1	D	211	LYS
1	D	319	ALA
1	A	177	GLY
1	A	456	ILE
1	A	467	GLU
1	B	177	GLY
1	B	335	ARG
1	B	456	ILE
1	C	177	GLY
1	C	299	ASP
1	C	409	ASP

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Mol	Chain	Res	Type
1	D	103	SER
1	D	177	GLY
1	D	409	ASP
1	D	456	ILE
1	A	323	LYS
1	A	434	ALA
1	B	299	ASP
1	B	409	ASP
1	B	434	ALA
1	C	467	GLU
1	D	323	LYS
1	D	467	GLU
1	A	300	CYS
1	C	300	CYS
1	C	323	LYS
1	C	434	ALA
1	C	460	LEU
1	D	434	ALA
1	B	467	GLU
1	C	273	PRO
1	C	320	PRO
1	D	273	PRO
1	A	320	PRO
1	A	460	LEU
1	A	408	PRO
1	D	370	GLY
1	D	375	ILE
1	A	436	PRO
1	B	320	PRO
1	B	408	PRO
1	D	408	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/385 (97%)	312 (84%)	61 (16%)	2	8
1	B	372/385 (97%)	310 (83%)	62 (17%)	2	7
1	C	372/385 (97%)	316 (85%)	56 (15%)	3	10
1	D	372/385 (97%)	318 (86%)	54 (14%)	3	10
All	All	1489/1540 (97%)	1256 (84%)	233 (16%)	2	9

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	30	LEU
1	A	33	CYS
1	A	34	GLN
1	A	41	ILE
1	A	54	LEU
1	A	101	GLU
1	A	103	SER
1	A	104	SER
1	A	106	LEU
1	A	124	VAL
1	A	130	SER
1	A	141	ASN
1	A	142	GLU
1	A	156	LYS
1	A	169	ASN
1	A	176	ASP
1	A	178	ARG
1	A	179	VAL
1	A	185	PRO
1	A	193	LEU
1	A	203	VAL
1	A	210	LEU
1	A	214	SER
1	A	218	ASN
1	A	220	GLU
1	A	226	ARG
1	A	228	LEU
1	A	241	THR
1	A	247	CYS

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Mol	Chain	Res	Type
1	A	248	THR
1	A	253	GLU
1	A	263	GLU
1	A	296	GLN
1	A	324	VAL
1	A	333	LYS
1	A	335	ARG
1	A	341	ARG
1	A	342	GLN
1	A	345	THR
1	A	351	TRP
1	A	353	GLU
1	A	362	LYS
1	A	372	GLU
1	A	379	ARG
1	A	385	ILE
1	A	390	THR
1	A	393	LYS
1	A	409	ASP
1	A	411	MSE
1	A	412	ASN
1	A	439	ASP
1	A	440	ASP
1	A	450	ILE
1	A	454	LYS
1	A	466	ARG
1	A	467	GLU
1	A	469	VAL
1	A	470	ARG
1	A	471	ASP
1	A	473	LYS
1	B	8	PHE
1	B	13	LEU
1	B	15	GLN
1	B	27	ASP
1	B	39	ARG
1	B	54	LEU
1	B	55	GLN
1	B	75	TRP
1	B	86	LEU
1	B	96	LEU
1	B	101	GLU

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Mol	Chain	Res	Type
1	B	103	SER
1	B	104	SER
1	B	112	PHE
1	B	124	VAL
1	B	131	LYS
1	B	135	ILE
1	B	141	ASN
1	B	142	GLU
1	B	153	SER
1	B	158	LEU
1	B	185	PRO
1	B	196	PRO
1	B	210	LEU
1	B	216	GLU
1	B	219	GLN
1	B	228	LEU
1	B	237	ARG
1	B	252	GLU
1	B	262	LYS
1	B	273	PRO
1	B	283	LYS
1	B	296	GLN
1	B	315	PRO
1	B	321	LYS
1	B	330	SER
1	B	335	ARG
1	B	336	GLU
1	B	342	GLN
1	B	345	THR
1	B	350	ASN
1	B	351	TRP
1	B	353	GLU
1	B	357	LEU
1	B	360	ARG
1	B	362	LYS
1	B	379	ARG
1	B	381	SER
1	B	386	LYS
1	B	405	LEU
1	B	412	ASN
1	B	433	GLN
1	B	440	ASP

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Mol	Chain	Res	Type
1	B	443	VAL
1	B	450	ILE
1	B	456	ILE
1	B	459	ARG
1	B	462	ASN
1	B	467	GLU
1	B	469	VAL
1	B	471	ASP
1	B	473	LYS
1	C	8	PHE
1	C	15	GLN
1	C	17	ARG
1	C	18	GLU
1	C	41	ILE
1	C	54	LEU
1	C	67	ILE
1	C	75	TRP
1	C	88	SER
1	C	96	LEU
1	C	101	GLU
1	C	103	SER
1	C	106	LEU
1	C	142	GLU
1	C	149	GLU
1	C	153	SER
1	C	154	ARG
1	C	156	LYS
1	C	163	SER
1	C	186	GLU
1	C	212	ASN
1	C	220	GLU
1	C	241	THR
1	C	250	ASN
1	C	251	GLN
1	C	273	PRO
1	C	296	GLN
1	C	322	TYR
1	C	323	LYS
1	C	324	VAL
1	C	326	ASN
1	C	330	SER
1	C	335	ARG

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Mol	Chain	Res	Type
1	C	341	ARG
1	C	342	GLN
1	C	345	THR
1	C	347	VAL
1	C	350	ASN
1	C	353	GLU
1	C	361	ASP
1	C	362	LYS
1	C	371	ILE
1	C	379	ARG
1	C	383	LEU
1	C	392	ASN
1	C	411	MSE
1	C	431	TYR
1	C	446	GLN
1	C	450	ILE
1	C	454	LYS
1	C	456	ILE
1	C	462	ASN
1	C	466	ARG
1	C	468	LEU
1	C	470	ARG
1	C	473	LYS
1	D	33	CYS
1	D	34	GLN
1	D	37	LEU
1	D	41	ILE
1	D	55	GLN
1	D	75	TRP
1	D	89	THR
1	D	101	GLU
1	D	104	SER
1	D	106	LEU
1	D	111	LEU
1	D	119	GLN
1	D	131	LYS
1	D	132	THR
1	D	149	GLU
1	D	167	ILE
1	D	178	ARG
1	D	179	VAL
1	D	185	PRO

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Mol	Chain	Res	Type
1	D	205	LYS
1	D	210	LEU
1	D	225	GLN
1	D	226	ARG
1	D	242	LEU
1	D	250	ASN
1	D	273	PRO
1	D	296	GLN
1	D	300	CYS
1	D	308	LEU
1	D	323	LYS
1	D	324	VAL
1	D	333	LYS
1	D	342	GLN
1	D	349	LEU
1	D	352	ASP
1	D	353	GLU
1	D	361	ASP
1	D	362	LYS
1	D	382	ARG
1	D	390	THR
1	D	409	ASP
1	D	411	MSE
1	D	412	ASN
1	D	415	GLU
1	D	419	GLN
1	D	439	ASP
1	D	440	ASP
1	D	446	GLN
1	D	450	ILE
1	D	462	ASN
1	D	467	GLU
1	D	470	ARG
1	D	471	ASP
1	D	473	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	134	GLN
1	A	141	ASN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	212	ASN
1	A	218	ASN
1	A	251	GLN
1	A	359	GLN
1	A	462	ASN
1	B	15	GLN
1	B	55	GLN
1	B	92	HIS
1	B	100	GLN
1	B	119	GLN
1	B	141	ASN
1	B	159	HIS
1	B	251	GLN
1	B	254	ASN
1	B	296	GLN
1	B	339	GLN
1	B	391	HIS
1	B	399	HIS
1	B	410	ASN
1	B	419	GLN
1	B	448	GLN
1	B	462	ASN
1	C	34	GLN
1	C	134	GLN
1	C	218	ASN
1	C	250	ASN
1	C	254	ASN
1	C	312	GLN
1	C	342	GLN
1	C	350	ASN
1	C	412	ASN
1	C	446	GLN
1	C	462	ASN
1	D	34	GLN
1	D	44	ASN
1	D	55	GLN
1	D	100	GLN
1	D	159	HIS
1	D	225	GLN
1	D	234	HIS
1	D	250	ASN

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Mol	Chain	Res	Type
1	D	254	ASN
1	D	296	GLN
1	D	410	ASN
1	D	433	GLN
1	D	447	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	448/479 (93%)	-1.31	0 100 100	52, 65, 70, 77	0
1	B	447/479 (93%)	-1.37	0 100 100	51, 65, 70, 76	0
1	C	447/479 (93%)	-1.36	0 100 100	51, 65, 70, 76	0
1	D	448/479 (93%)	-1.30	0 100 100	52, 65, 70, 76	0
All	All	1790/1916 (93%)	-1.34	0 100 100	51, 65, 70, 77	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.