



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:42 AM GMT

PDB ID : 2NVW
Title : Crystal structure of transcriptional regulator Gal80p from *Kluyveromyces fragilis*
Authors : Thoden, J.B.; Sellick, C.A.; Reece, R.J.; Holden, H.M.
Deposited on : 2006-11-13
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

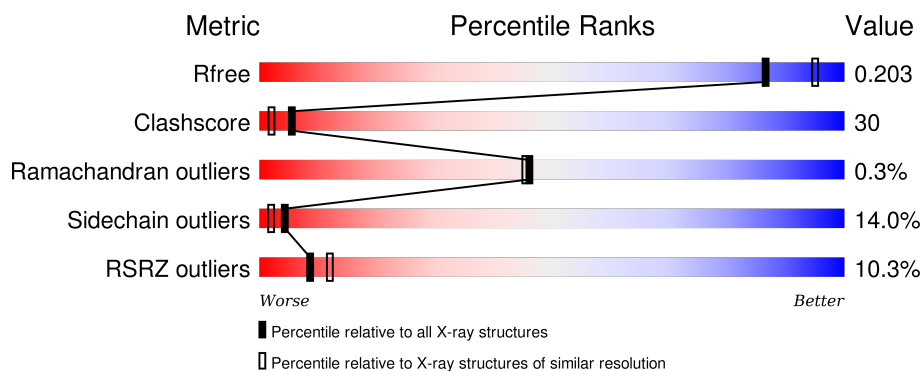
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>9%</div> <div>43%</div> <div>35%</div> <div>8%</div> <div>14%</div> </div>
1	B	479	<div> <div>9%</div> <div>39%</div> <div>35%</div> <div>10%</div> <div>15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6895 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	1	0
			3310	2117	563	620	10			
1	B	405	Total	C	N	O	S	0	0	0
			3238	2072	547	609	10			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	INITIATING METHIONINE	UNP Q06433
A	-20	GLY	-	CLONING ARTIFACT	UNP Q06433
A	-19	SER	-	CLONING ARTIFACT	UNP Q06433
A	-18	SER	-	CLONING ARTIFACT	UNP Q06433
A	-17	HIS	-	EXPRESSION TAG	UNP Q06433
A	-16	HIS	-	EXPRESSION TAG	UNP Q06433
A	-15	HIS	-	EXPRESSION TAG	UNP Q06433
A	-14	HIS	-	EXPRESSION TAG	UNP Q06433
A	-13	HIS	-	EXPRESSION TAG	UNP Q06433
A	-12	HIS	-	EXPRESSION TAG	UNP Q06433
A	-11	SER	-	CLONING ARTIFACT	UNP Q06433
A	-10	SER	-	CLONING ARTIFACT	UNP Q06433
A	-9	GLU	-	CLONING ARTIFACT	UNP Q06433
A	-8	ASN	-	CLONING ARTIFACT	UNP Q06433
A	-7	LEU	-	CLONING ARTIFACT	UNP Q06433
A	-6	TYR	-	CLONING ARTIFACT	UNP Q06433
A	-5	PHE	-	CLONING ARTIFACT	UNP Q06433
A	-4	GLN	-	CLONING ARTIFACT	UNP Q06433
A	-3	GLY	-	CLONING ARTIFACT	UNP Q06433
A	-2	HIS	-	CLONING ARTIFACT	UNP Q06433
A	-1	MET	-	CLONING ARTIFACT	UNP Q06433
A	0	LEU	-	CLONING ARTIFACT	UNP Q06433
A	1	ALA	-	CLONING ARTIFACT	UNP Q06433
B	-21	MET	-	INITIATING METHIONINE	UNP Q06433
B	-20	GLY	-	CLONING ARTIFACT	UNP Q06433

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	CLONING ARTIFACT	UNP Q06433
B	-18	SER	-	CLONING ARTIFACT	UNP Q06433
B	-17	HIS	-	EXPRESSION TAG	UNP Q06433
B	-16	HIS	-	EXPRESSION TAG	UNP Q06433
B	-15	HIS	-	EXPRESSION TAG	UNP Q06433
B	-14	HIS	-	EXPRESSION TAG	UNP Q06433
B	-13	HIS	-	EXPRESSION TAG	UNP Q06433
B	-12	HIS	-	EXPRESSION TAG	UNP Q06433
B	-11	SER	-	CLONING ARTIFACT	UNP Q06433
B	-10	SER	-	CLONING ARTIFACT	UNP Q06433
B	-9	GLU	-	CLONING ARTIFACT	UNP Q06433
B	-8	ASN	-	CLONING ARTIFACT	UNP Q06433
B	-7	LEU	-	CLONING ARTIFACT	UNP Q06433
B	-6	TYR	-	CLONING ARTIFACT	UNP Q06433
B	-5	PHE	-	CLONING ARTIFACT	UNP Q06433
B	-4	GLN	-	CLONING ARTIFACT	UNP Q06433
B	-3	GLY	-	CLONING ARTIFACT	UNP Q06433
B	-2	HIS	-	CLONING ARTIFACT	UNP Q06433
B	-1	MET	-	CLONING ARTIFACT	UNP Q06433
B	0	LEU	-	CLONING ARTIFACT	UNP Q06433
B	1	ALA	-	CLONING ARTIFACT	UNP Q06433

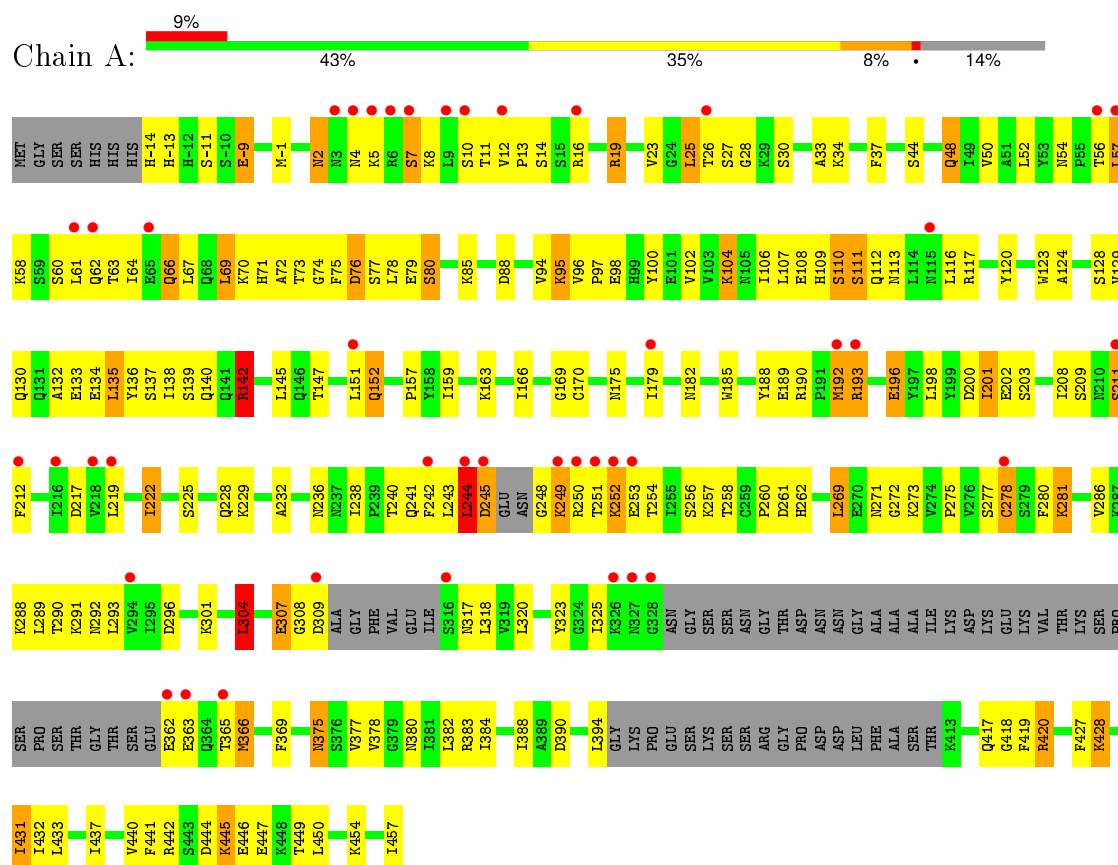
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	203	Total 203	O 203	0	0
2	B	144	Total 144	O 144	0	0

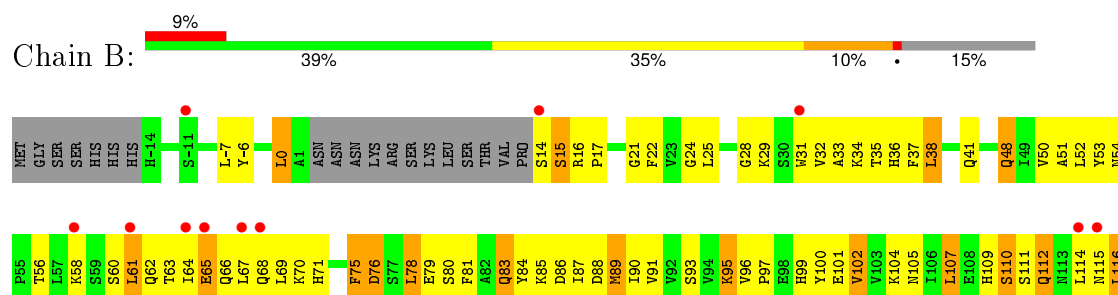
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Galactose/lactose metabolism regulatory protein GAL80



- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80



R420	F421	E422	K428	D429	A430	I431	I432	I433	H434	R435	I436	I437	D438	F441	R442	K445	E446	E447	K448	T449	I450	D451	V452	S453	K454	I455	M456	I457																								
GLU	LYS	VAL	THR	LYS	SER	PRO	PRO	SER	THR	GLY	THR	SER	E361	E362	T365	M366	F369	R372	N375	N380	R383	I384	S387	F393	L394	G395	LYS	PRO	GLU	SER	LYS	SER	SER	ARG	GLY	PRO	ASP	ASP	LEU	PHE	ALA	SER	THR	K413	F414	D415	K416	Q417	G418	F419		
F280	K281	T284	F285	V286	K287	K288	L289	N292	L293	V294	L295	D296	I297	G299	T300	K301	L304	D309	A310	G311	PHE	VAL	GLU	ILE	S316	V319	L320	Y321	F322	G323	G324	I325	K326	N327	G328	ASN	GLY	SER	SER	ASP	ASN	GLY	THR	ASP	ASN	GLY	ALA	ALA	ILE	LYS	ASP	LYS
E189	R190	P191	M192	R193	S194	P195	E196	Y197	L198	Y199	D200	I201	E202	S203	D236	I237	D217	V218	L219	Q220	Y221	I222	F227	Q228	K229	L151	A232	N236	F242	L243	L244	D245	E246	N247	GLY	LVS	R250	T251	K252	E253	T254	I255	S256	K257	T258	C259	I259	D261	L264	C278	S279	Y188
R117	Y120	Y121	E122	H123	A124	L125	A126	A127	S128	V129	Q130	Q131	A132	E133	E134	L135	Y136	S137	I138	S139	Q140	Q141	R142	L145	I149	C150	L151	Q152	G153	R154	K155	S156	P157	Y158	I159	V160	K163	E164	L165	I166	S167	D173	S176	I177	E178	I179	G183	G184	W185	Y186	G187	Y188

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.20 Å 137.10 Å 72.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 37.30 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.10) 97.4 (37.30-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.08 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.195 , 0.245 0.199 , 0.203	Depositor DCC
R_{free} test set	6516 reflections (11.16%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 112.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 65500 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6895	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	0/3381	1.50	34/4560 (0.7%)
1	B	0.79	1/3302 (0.0%)	1.52	41/4453 (0.9%)
All	All	0.78	1/6683 (0.0%)	1.51	75/9013 (0.8%)

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	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	GLU	CB-CG	5.55	1.62	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	LEU	CB-CG-CD1	-9.85	94.25	111.00
1	A	145	LEU	CB-CG-CD2	-9.68	94.54	111.00
1	B	219	LEU	CA-CB-CG	-9.24	94.06	115.30
1	B	435	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	A	296	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	A	244	LEU	CB-CG-CD1	-8.06	97.30	111.00
1	B	436	LEU	CB-CG-CD2	-7.82	97.70	111.00
1	A	88	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	B	154	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	145	LEU	CB-CG-CD2	-7.09	98.94	111.00
1	B	135	LEU	CA-CB-CG	-7.03	99.12	115.30
1	A	78	LEU	CB-CG-CD2	-6.99	99.11	111.00
1	A	222	ILE	CB-CA-C	-6.95	97.70	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	LEU	CA-CB-CG	-6.95	99.32	115.30
1	A	198	LEU	CB-CG-CD1	-6.87	99.33	111.00
1	A	269	LEU	CB-CG-CD1	-6.86	99.34	111.00
1	B	229	LYS	CB-CA-C	-6.85	96.70	110.40
1	B	142	ARG	CB-CA-C	6.77	123.95	110.40
1	A	258	THR	CA-CB-CG2	-6.59	103.18	112.40
1	A	72	ALA	N-CA-C	6.53	128.63	111.00
1	B	107	LEU	CA-CB-CG	-6.51	100.33	115.30
1	B	76	ASP	N-CA-CB	-6.44	99.01	110.60
1	B	0	LEU	CA-CB-CG	-6.38	100.61	115.30
1	A	-14	HIS	N-CA-C	6.36	128.16	111.00
1	B	293	LEU	CA-CB-CG	-6.27	100.87	115.30
1	A	52	LEU	CB-CA-C	-6.15	98.52	110.20
1	B	65	GLU	CA-CB-CG	6.01	126.63	113.40
1	A	112	GLN	CB-CA-C	5.93	122.27	110.40
1	A	307	GLU	N-CA-CB	-5.93	99.92	110.60
1	A	135	LEU	CA-CB-CG	-5.93	101.66	115.30
1	A	304	LEU	CB-CG-CD1	-5.92	100.94	111.00
1	A	244	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	B	442	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	B	61	LEU	CA-CB-CG	-5.86	101.83	115.30
1	A	52	LEU	CB-CG-CD1	-5.85	101.05	111.00
1	A	185	TRP	CB-CA-C	-5.83	98.73	110.40
1	A	277	SER	N-CA-CB	5.81	119.22	110.50
1	A	112	GLN	N-CA-CB	5.80	121.05	110.60
1	B	-7	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	A	-1	MET	CG-SD-CE	5.76	109.42	100.20
1	A	420	ARG	CG-CD-NE	-5.67	99.89	111.80
1	A	95	LYS	CB-CA-C	-5.65	99.11	110.40
1	A	252	LYS	CD-CE-NZ	-5.63	98.75	111.70
1	B	114	LEU	CB-CG-CD2	-5.60	101.47	111.00
1	B	296	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	420	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	449	THR	N-CA-C	-5.46	96.25	111.00
1	B	78	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	A	142	ARG	CA-CB-CG	-5.43	101.45	113.40
1	A	135	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	B	22	PHE	CB-CA-C	-5.39	99.62	110.40
1	B	151	LEU	N-CA-C	-5.38	96.49	111.00
1	A	252	LYS	N-CA-C	-5.35	96.56	111.00
1	A	382	LEU	CB-CG-CD1	5.33	120.07	111.00
1	B	129	VAL	CB-CA-C	-5.33	101.27	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	B	447	GLU	CB-CA-C	-5.23	99.94	110.40
1	B	393	PHE	CB-CG-CD1	-5.22	117.14	120.80
1	A	457	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	A	151	LEU	N-CA-C	-5.19	96.98	111.00
1	B	198	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	B	372	ARG	C-N-CA	-5.16	108.79	121.70
1	B	289	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	A	363	GLU	N-CA-C	-5.13	97.14	111.00
1	B	76	ASP	CB-CA-C	-5.13	100.13	110.40
1	B	190	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	B	89	MET	CB-CA-C	-5.11	100.17	110.40
1	B	222	ILE	CG1-CB-CG2	5.11	122.64	111.40
1	B	258	THR	N-CA-CB	-5.10	100.61	110.30
1	B	296	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	217	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	375	ASN	N-CA-C	-5.06	97.35	111.00
1	B	38	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	B	186	TYR	N-CA-C	5.03	124.58	111.00
1	B	65	GLU	N-CA-CB	-5.01	101.57	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	112	GLN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ASN	Mainchain

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	3310	0	3309	172	1
1	B	3238	0	3218	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	203	0	0	15	0
2	B	144	0	0	7	1
All	All	6895	0	6527	387	1

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 30.

All (387) 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:251:THR:HG22	1:A:253:GLU:H	1.06	1.15
1:B:25:LEU:HD23	1:B:52:LEU:HD21	1.36	1.07
1:B:159:ILE:HG23	1:B:222:ILE:HD11	1.38	1.04
1:A:70:LYS:HG3	1:A:71:HIS:CD2	1.98	0.99
1:A:250:ARG:HG2	1:A:251:THR:H	1.26	0.98
1:B:152:GLN:HE21	1:B:152:GLN:H	1.15	0.94
1:B:152:GLN:H	1:B:152:GLN:NE2	1.66	0.94
1:B:136:TYR:HB2	1:B:431:ILE:HD13	1.48	0.93
1:A:152:GLN:HE21	1:A:152:GLN:H	1.01	0.93
1:B:251:THR:HG22	1:B:253:GLU:H	1.35	0.92
1:A:251:THR:CG2	1:A:253:GLU:H	1.83	0.91
1:B:152:GLN:HA	1:B:384:ILE:HD11	1.53	0.91
1:A:136:TYR:HB2	1:A:431:ILE:HD11	1.56	0.88
1:A:95:LYS:HB3	1:A:97:PRO:HD2	1.57	0.86
1:A:192:MET:SD	1:A:245:ASP:HB2	2.16	0.86
1:A:251:THR:HG22	1:A:253:GLU:N	1.89	0.86
1:B:159:ILE:HG23	1:B:222:ILE:CD1	2.06	0.85
1:A:26:THR:HB	1:A:30:SER:HB3	1.59	0.84
1:A:301:LYS:HD2	1:A:325:ILE:HD13	1.60	0.83
1:A:152:GLN:H	1:A:152:GLN:NE2	1.76	0.83
1:A:375:ASN:OD1	1:A:377:VAL:HG12	1.79	0.83
1:B:251:THR:HG21	1:B:253:GLU:HG3	1.62	0.81
1:B:138:ILE:O	1:B:141:GLN:HB2	1.81	0.80
1:B:123:TRP:CD2	1:B:124:ALA:HA	2.17	0.80
1:B:159:ILE:HG13	1:B:222:ILE:CD1	2.12	0.80
1:B:152:GLN:N	1:B:152:GLN:HE21	1.79	0.79
1:B:136:TYR:CB	1:B:431:ILE:HD13	2.12	0.79
1:B:159:ILE:CG2	1:B:222:ILE:HD11	2.11	0.79
1:B:192:MET:SD	1:B:245:ASP:HB2	2.23	0.78
1:A:309:ASP:HB3	2:A:633:HOH:O	1.83	0.78
1:A:309:ASP:OD1	1:A:317:ASN:HB2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:THR:HG22	1:B:252:LYS:N	1.99	0.77
1:A:192:MET:CE	1:A:245:ASP:HB2	2.14	0.77
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.20	0.77
1:B:54:ASN:HB2	1:B:60:SER:OG	1.84	0.76
1:B:128:SER:OG	1:B:130:GLN:HG2	1.85	0.76
1:A:152:GLN:HE21	1:A:152:GLN:N	1.81	0.75
1:B:185:TRP:NE1	2:B:530:HOH:O	2.19	0.75
1:A:251:THR:HG22	1:A:252:LYS:H	1.51	0.75
1:A:251:THR:HG22	1:A:252:LYS:N	2.01	0.75
1:B:428:LYS:O	1:B:428:LYS:HD2	1.87	0.75
1:B:201:ILE:HB	1:B:258:THR:HG22	1.68	0.75
1:B:451:ASP:OD1	1:B:453:SER:HB2	1.87	0.74
1:A:428:LYS:HD2	1:A:428:LYS:O	1.87	0.74
1:B:84:TYR:CE1	1:B:86:ASP:HB2	2.22	0.74
1:B:79:GLU:O	1:B:83:GLN:NE2	2.20	0.74
1:B:455:ILE:HG12	1:B:456:MET:CE	2.17	0.73
1:B:159:ILE:HG13	1:B:222:ILE:HD11	1.69	0.73
1:A:250:ARG:HG2	1:A:251:THR:N	2.00	0.73
1:A:136:TYR:HB2	1:A:431:ILE:CD1	2.19	0.73
1:A:70:LYS:HG3	1:A:71:HIS:HD2	1.53	0.73
1:B:200:ASP:OD1	1:B:201:ILE:N	2.23	0.72
1:B:257:LYS:HD2	1:B:259:CYS:O	1.90	0.72
1:A:67:LEU:HB2	1:A:69:LEU:HD21	1.72	0.72
1:A:420:ARG:HD2	2:A:608:HOH:O	1.90	0.71
1:B:441:PHE:O	1:B:445:LYS:HG3	1.91	0.71
1:B:431:ILE:O	1:B:435:ARG:HG3	1.91	0.71
1:B:58:LYS:HD3	2:B:491:HOH:O	1.90	0.70
1:A:245:ASP:OD1	1:A:249:LYS:NZ	2.23	0.70
1:A:-11:SER:HB3	1:A:-9:GLU:HG3	1.73	0.70
1:B:107:LEU:O	1:B:142:ARG:NH2	2.25	0.69
1:A:308:GLY:HA3	1:A:318:LEU:HD23	1.74	0.69
1:B:88:ASP:O	1:B:116:LEU:HD12	1.93	0.69
1:B:451:ASP:OD1	1:B:453:SER:N	2.26	0.69
1:B:251:THR:CG2	1:B:253:GLU:H	2.07	0.68
1:A:201:ILE:HD12	1:A:201:ILE:O	1.93	0.68
1:A:2:ASN:HB3	1:A:4:ASN:H	1.57	0.67
1:A:380:ASN:HB2	2:A:655:HOH:O	1.93	0.67
1:A:4:ASN:O	1:A:10:SER:HB3	1.95	0.67
1:A:442:ARG:NH2	2:A:536:HOH:O	2.28	0.67
1:B:251:THR:HG22	1:B:252:LYS:H	1.60	0.67
1:B:455:ILE:HG12	1:B:456:MET:HE1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:HG13	1:A:378:VAL:N	2.10	0.66
1:A:286:VAL:HG13	1:A:292:ASN:ND2	2.11	0.66
2:A:612:HOH:O	1:B:448:LYS:HD3	1.95	0.66
1:B:25:LEU:CD2	1:B:52:LEU:HD21	2.21	0.65
1:A:12:VAL:HB	1:A:13:PRO:HD3	1.79	0.65
1:B:130:GLN:H	1:B:130:GLN:CD	1.98	0.65
1:B:36:HIS:NE2	1:B:122:GLU:OE2	2.22	0.65
1:B:251:THR:CG2	1:B:253:GLU:HG3	2.26	0.65
1:A:196:GLU:H	1:A:196:GLU:CD	1.98	0.64
1:B:31:TRP:CH2	1:B:35:THR:HG21	2.32	0.64
1:B:31:TRP:CZ2	1:B:35:THR:HG21	2.33	0.64
1:A:269:LEU:O	1:A:273:LYS:HA	1.97	0.64
1:A:251:THR:HG21	1:A:253:GLU:HB2	1.79	0.64
1:A:106:ILE:O	1:A:110:SER:OG	2.16	0.64
1:B:136:TYR:HB2	1:B:431:ILE:CD1	2.23	0.63
1:B:435:ARG:HD2	1:B:455:ILE:O	1.97	0.63
1:B:251:THR:HG22	1:B:253:GLU:N	2.11	0.63
1:A:228:GLN:NE2	1:A:273:LYS:HE3	2.14	0.63
1:A:249:LYS:NZ	1:A:249:LYS:HB3	2.14	0.63
1:A:290:THR:HA	2:A:511:HOH:O	1.97	0.63
1:A:241:GLN:HA	2:A:495:HOH:O	1.98	0.62
1:B:183:GLY:HA3	1:B:207:LEU:CD1	2.28	0.62
1:B:95:LYS:CG	1:B:97:PRO:HD2	2.29	0.62
1:A:26:THR:HG22	1:A:27:SER:N	2.13	0.62
1:B:80:SER:HA	1:B:83:GLN:NE2	2.15	0.62
1:A:57:LEU:HD23	1:A:61:LEU:CD1	2.29	0.62
1:B:163:LYS:HE3	1:B:221:TYR:CZ	2.34	0.62
1:B:192:MET:CE	1:B:245:ASP:HB2	2.30	0.62
1:A:317:ASN:HB3	2:A:660:HOH:O	2.00	0.62
1:B:201:ILE:CB	1:B:258:THR:HG22	2.30	0.61
1:A:110:SER:HB3	1:A:116:LEU:HD22	1.80	0.61
1:B:79:GLU:HG3	1:B:109:HIS:CE1	2.35	0.61
1:A:377:VAL:CG1	1:A:378:VAL:N	2.63	0.61
1:A:102:VAL:O	1:A:106:ILE:HD12	2.00	0.60
1:B:323:TYR:CD1	1:B:366:MET:HG2	2.36	0.60
1:B:123:TRP:HA	1:B:149:ILE:HD11	1.82	0.60
1:B:85:LYS:O	1:B:115:ASN:ND2	2.34	0.60
1:A:28:GLY:HA2	1:A:67:LEU:HD21	1.84	0.60
1:B:96:VAL:N	1:B:97:PRO:CD	2.65	0.60
1:B:16:ARG:HG2	1:B:17:PRO:O	2.02	0.60
1:B:195:PRO:HB2	1:B:197:TYR:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ILE:HG22	1:B:258:THR:CG2	2.32	0.59
1:B:159:ILE:CG1	1:B:222:ILE:HD11	2.33	0.59
1:B:284:THR:HB	1:B:285:PRO:HA	1.84	0.59
1:B:84:TYR:CZ	1:B:86:ASP:HB2	2.38	0.58
1:B:188:TYR:HD1	1:B:285:PRO:HD3	1.67	0.58
1:A:79:GLU:HG3	1:A:109:HIS:CG	2.38	0.58
1:A:377:VAL:HG13	1:A:378:VAL:HG23	1.85	0.58
1:B:200:ASP:OD1	1:B:200:ASP:C	2.39	0.58
1:B:251:THR:CG2	1:B:252:LYS:N	2.65	0.58
1:B:301:LYS:HB3	1:B:325:ILE:HD13	1.86	0.58
1:B:301:LYS:HD3	1:B:325:ILE:HD12	1.86	0.58
1:B:64:ILE:O	1:B:69:LEU:N	2.28	0.58
1:B:197:TYR:CZ	1:B:198:LEU:HD21	2.39	0.57
1:A:242:PHE:CG	1:A:250:ARG:HD3	2.40	0.57
1:A:390:ASP:HA	1:A:394:LEU:HD12	1.86	0.57
1:B:105:ASN:OD1	1:B:105:ASN:C	2.42	0.57
1:B:433:LEU:O	1:B:437:ILE:HD12	2.05	0.57
1:A:244:LEU:HB3	1:A:249:LYS:O	2.05	0.57
1:B:33:ALA:O	1:B:37:PHE:HB3	2.05	0.57
1:B:250:ARG:HG2	1:B:251:THR:N	2.20	0.56
1:B:123:TRP:CG	1:B:124:ALA:HA	2.39	0.56
1:A:134:GLU:HA	1:A:137:SER:OG	2.05	0.56
1:B:455:ILE:HG12	1:B:456:MET:HE3	1.85	0.56
1:A:200:ASP:OD1	1:A:202:GLU:HB2	2.05	0.56
1:B:159:ILE:CB	1:B:222:ILE:HD11	2.35	0.56
1:B:31:TRP:CE2	1:B:35:THR:HG21	2.41	0.56
1:A:236:ASN:ND2	1:A:260:PRO:HA	2.20	0.56
1:B:432:ILE:HG12	1:B:456:MET:HA	1.88	0.56
1:A:26:THR:HB	1:A:30:SER:CB	2.35	0.56
1:B:25:LEU:HD13	1:B:32:VAL:HG12	1.89	0.55
1:A:325:ILE:HG13	1:A:325:ILE:O	2.06	0.55
1:B:127:ALA:HB1	1:B:203:SER:O	2.06	0.55
1:B:115:ASN:O	1:B:117:ARG:HG3	2.06	0.55
1:B:31:TRP:O	1:B:35:THR:N	2.39	0.55
1:A:62:GLN:O	1:A:66:GLN:HG3	2.06	0.55
1:A:13:PRO:HA	1:A:16:ARG:NH1	2.22	0.55
1:B:173:ASP:O	1:B:299:GLY:HA2	2.06	0.55
1:A:169:GLY:O	1:A:325:ILE:HD11	2.07	0.55
1:B:199:TYR:HD2	1:B:257:LYS:HG3	1.70	0.55
1:B:126:ALA:HB3	1:B:132:ALA:HB2	1.89	0.54
1:A:320:LEU:C	1:A:320:LEU:HD23	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HD23	1:B:52:LEU:CD2	2.25	0.54
1:B:95:LYS:HG2	1:B:97:PRO:HD2	1.88	0.54
1:B:301:LYS:HD3	1:B:325:ILE:CD1	2.38	0.54
1:A:304:LEU:HD23	1:A:304:LEU:C	2.28	0.54
1:A:209:SER:HA	1:A:437:ILE:HD13	1.89	0.54
1:B:187:GLY:HA3	1:B:284:THR:O	2.07	0.54
1:B:384:ILE:O	1:B:387:SER:HB2	2.08	0.54
2:A:512:HOH:O	1:B:287:LYS:HG2	2.08	0.54
1:B:24:GLY:HA3	1:B:93:SER:O	2.07	0.54
1:A:108:GLU:O	1:A:111:SER:OG	2.24	0.54
1:B:67:LEU:HD23	1:B:67:LEU:N	2.23	0.54
1:A:12:VAL:CB	1:A:13:PRO:HD3	2.37	0.53
1:A:-13:HIS:O	1:A:-13:HIS:HD2	1.90	0.53
1:B:189:GLU:HB3	1:B:244:LEU:HD21	1.89	0.53
1:B:185:TRP:HB3	1:B:199:TYR:OH	2.07	0.53
1:A:2:ASN:HD22	1:A:7:SER:HG	1.54	0.53
1:A:133:GLU:O	1:A:136:TYR:HB3	2.08	0.53
1:B:149:ILE:HG13	1:B:430:ALA:HB2	1.90	0.53
1:B:323:TYR:HD1	1:B:366:MET:HG2	1.72	0.53
1:A:100:TYR:OH	1:A:104:LYS:HE3	2.08	0.53
1:B:320:LEU:HB3	1:B:369:PHE:HB3	1.90	0.53
1:B:100:TYR:OH	1:B:134:GLU:OE1	2.23	0.53
1:B:454:LYS:NZ	2:B:563:HOH:O	2.42	0.53
1:B:244:LEU:HD23	1:B:250:ARG:HG3	1.91	0.52
1:B:14:SER:O	1:B:16:ARG:N	2.42	0.52
1:A:262:HIS:CE1	1:A:281:LYS:HG3	2.44	0.52
1:B:201:ILE:CG2	1:B:258:THR:HG22	2.40	0.52
1:A:128:SER:HB2	1:A:130:GLN:OE1	2.09	0.52
1:A:33:ALA:O	1:A:37:PHE:HB3	2.09	0.52
1:B:201:ILE:HD12	1:B:201:ILE:O	2.10	0.52
1:B:50:VAL:HA	1:B:71:HIS:O	2.10	0.52
1:B:67:LEU:O	1:B:68:GLN:HB2	2.09	0.51
1:A:192:MET:HE1	1:A:245:ASP:HB2	1.92	0.51
1:B:163:LYS:HE3	1:B:221:TYR:CE2	2.46	0.51
1:A:100:TYR:O	1:A:104:LYS:HB2	2.09	0.51
1:B:319:VAL:HG11	1:B:321:TYR:CZ	2.45	0.51
1:B:251:THR:CG2	1:B:252:LYS:H	2.22	0.51
1:B:128:SER:HG	1:B:130:GLN:HG2	1.76	0.51
1:A:102:VAL:HG12	1:A:106:ILE:HD12	1.92	0.51
1:A:251:THR:HG21	1:A:253:GLU:CB	2.41	0.50
1:A:79:GLU:HG3	1:A:109:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:CE1	1:B:300:THR:HG22	2.46	0.50
1:A:244:LEU:HB3	1:A:249:LYS:C	2.31	0.50
1:B:31:TRP:CZ3	1:B:35:THR:HG21	2.46	0.50
1:B:320:LEU:C	1:B:320:LEU:HD23	2.31	0.50
1:B:431:ILE:O	1:B:435:ARG:CG	2.59	0.50
1:A:134:GLU:O	1:A:137:SER:OG	2.27	0.50
1:B:455:ILE:CG1	1:B:456:MET:HE3	2.42	0.50
1:B:199:TYR:CD1	1:B:199:TYR:N	2.78	0.50
1:B:451:ASP:CG	1:B:453:SER:HB2	2.32	0.50
1:A:157:PRO:HG3	1:A:383:ARG:NH1	2.27	0.50
1:A:70:LYS:HE3	1:A:71:HIS:NE2	2.27	0.50
1:B:34:LYS:O	1:B:38:LEU:HD12	2.12	0.50
1:A:8:LYS:O	1:A:14:SER:OG	2.27	0.50
1:B:35:THR:OG1	1:B:36:HIS:N	2.39	0.50
1:B:325:ILE:C	1:B:327:ASN:H	2.15	0.50
1:B:37:PHE:O	1:B:41:GLN:HB2	2.11	0.50
1:B:228:GLN:HE21	1:B:229:LYS:HB2	1.76	0.50
1:B:236:ASN:HA	1:B:261:ASP:OD1	2.12	0.50
1:A:63:THR:HA	1:A:66:GLN:OE1	2.12	0.49
1:A:323:TYR:HA	1:A:365:THR:O	2.12	0.49
1:B:428:LYS:C	1:B:428:LYS:HD2	2.27	0.49
1:A:102:VAL:HG12	1:A:106:ILE:CD1	2.43	0.49
1:A:79:GLU:HB2	2:A:475:HOH:O	2.12	0.49
1:B:200:ASP:O	1:B:203:SER:OG	2.28	0.49
1:A:384:ILE:O	1:A:388:ILE:HG13	2.13	0.49
1:A:73:THR:HG22	1:A:74:GLY:N	2.27	0.49
1:A:159:ILE:CD1	1:A:159:ILE:N	2.75	0.49
1:B:48:GLN:HB2	2:B:580:HOH:O	2.12	0.49
1:B:201:ILE:H	1:B:258:THR:CG2	2.26	0.48
1:B:37:PHE:O	1:B:41:GLN:N	2.44	0.48
1:B:120:TYR:C	1:B:120:TYR:HD2	2.16	0.48
1:B:96:VAL:N	1:B:97:PRO:HD3	2.27	0.48
1:A:57:LEU:CD2	1:A:61:LEU:HD11	2.44	0.48
1:A:375:ASN:HB2	2:A:607:HOH:O	2.13	0.48
1:A:48:GLN:OE1	1:A:71:HIS:CD2	2.66	0.48
1:A:26:THR:HG22	1:A:27:SER:CB	2.43	0.48
1:B:110:SER:HB2	1:B:142:ARG:HH12	1.79	0.48
1:A:260:PRO:HD2	2:A:498:HOH:O	2.14	0.48
1:B:75:PHE:N	1:B:75:PHE:CD1	2.80	0.48
1:A:365:THR:CG2	1:A:366:MET:N	2.77	0.48
1:B:129:VAL:HG21	1:B:438:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:HB2	2:B:535:HOH:O	2.14	0.48
1:A:175:ASN:O	1:A:275:PRO:HD2	2.14	0.48
1:A:94:VAL:O	1:A:95:LYS:C	2.51	0.48
1:A:232:ALA:CB	1:A:440:VAL:HG13	2.44	0.48
1:A:4:ASN:O	1:A:7:SER:HB3	2.14	0.48
1:A:107:LEU:HD13	1:A:138:ILE:CG2	2.43	0.48
1:B:188:TYR:CD1	1:B:285:PRO:HD3	2.48	0.48
1:B:112:GLN:HG2	2:B:581:HOH:O	2.14	0.48
1:A:96:VAL:N	1:A:97:PRO:CD	2.76	0.47
1:B:128:SER:CB	1:B:130:GLN:HG2	2.44	0.47
1:A:139:SER:O	1:A:140:GLN:C	2.51	0.47
1:B:244:LEU:CD2	1:B:250:ARG:HG3	2.45	0.47
1:B:120:TYR:C	1:B:120:TYR:CD2	2.87	0.47
1:A:249:LYS:HB3	1:A:249:LYS:HZ2	1.78	0.47
1:A:129:VAL:O	1:A:133:GLU:HG2	2.15	0.47
1:B:325:ILE:C	1:B:327:ASN:N	2.65	0.47
1:B:155:LYS:O	1:B:383:ARG:NH1	2.40	0.47
1:B:100:TYR:HB2	1:B:131:GLN:OE1	2.15	0.47
1:B:116:LEU:HA	1:B:116:LEU:HD12	1.50	0.47
1:A:123:TRP:CE3	1:A:124:ALA:HA	2.50	0.46
1:B:14:SER:C	1:B:16:ARG:H	2.18	0.46
1:A:286:VAL:HG13	1:A:292:ASN:HD21	1.80	0.46
1:B:95:LYS:C	1:B:97:PRO:HD2	2.35	0.46
1:B:177:ILE:HG12	1:B:297:ILE:HG12	1.97	0.46
1:A:238:ILE:O	1:A:238:ILE:HG22	2.14	0.46
1:A:257:LYS:HB3	1:A:257:LYS:HE3	1.62	0.46
1:A:27:SER:HA	1:A:63:THR:OG1	2.16	0.46
1:B:28:GLY:HA3	1:B:66:GLN:OE1	2.15	0.46
1:A:225:SER:HB2	1:A:271:ASN:ND2	2.31	0.46
1:B:441:PHE:O	1:B:445:LYS:CG	2.61	0.46
1:B:96:VAL:HA	1:B:99:HIS:CD2	2.51	0.46
1:B:135:LEU:HA	1:B:135:LEU:HD23	1.67	0.46
1:A:95:LYS:HB2	1:A:98:GLU:OE1	2.16	0.46
1:B:21:GLY:HA2	1:B:51:ALA:O	2.16	0.46
1:A:193:ARG:HD2	1:A:193:ARG:HA	1.62	0.46
1:A:290:THR:HG23	2:A:510:HOH:O	2.15	0.45
1:B:136:TYR:CB	1:B:431:ILE:CD1	2.91	0.45
1:B:65:GLU:O	1:B:68:GLN:N	2.49	0.45
1:B:152:GLN:CA	1:B:384:ILE:HD11	2.35	0.45
1:B:14:SER:C	1:B:16:ARG:N	2.69	0.45
1:A:25:LEU:C	1:A:25:LEU:HD12	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLN:N	1:B:130:GLN:CD	2.67	0.45
1:A:57:LEU:HD23	1:A:61:LEU:HD11	1.97	0.45
1:B:325:ILE:O	1:B:325:ILE:HG12	2.17	0.45
1:B:63:THR:HA	1:B:66:GLN:NE2	2.32	0.45
1:B:422:GLU:H	1:B:422:GLU:CD	2.19	0.45
1:A:289:LEU:HD21	1:B:323:TYR:HB2	1.98	0.45
1:A:-13:HIS:O	1:A:-13:HIS:CD2	2.70	0.45
1:A:229:LYS:HD2	1:A:449:THR:HG21	1.99	0.45
1:B:136:TYR:CG	1:B:431:ILE:HD13	2.52	0.44
1:B:201:ILE:HG22	1:B:258:THR:HG21	1.99	0.44
1:B:62:GLN:C	1:B:66:GLN:HE21	2.20	0.44
1:A:244:LEU:HA	1:A:249:LYS:O	2.18	0.44
1:A:166:ILE:HD12	1:A:222:ILE:HG22	1.98	0.44
1:A:441:PHE:O	1:A:445:LYS:N	2.47	0.44
1:A:377:VAL:CG1	1:A:378:VAL:HG23	2.48	0.44
1:A:229:LYS:HA	1:A:450:LEU:O	2.18	0.44
1:A:57:LEU:O	1:A:61:LEU:HD13	2.17	0.44
1:A:60:SER:O	1:A:64:ILE:HG13	2.18	0.44
1:B:195:PRO:O	1:B:196:GLU:C	2.54	0.44
1:B:66:GLN:C	1:B:68:GLN:H	2.21	0.44
1:B:259:CYS:HA	1:B:260:PRO:HD3	1.79	0.44
1:B:292:ASN:HB2	1:B:310:ALA:HB3	1.99	0.44
1:A:67:LEU:CB	1:A:69:LEU:HD21	2.46	0.43
1:B:88:ASP:C	1:B:116:LEU:HD12	2.38	0.43
1:B:195:PRO:CB	1:B:197:TYR:CD2	3.01	0.43
1:B:165:LEU:HD21	1:B:326:LYS:HE3	2.01	0.43
1:A:272:GLY:O	1:A:273:LYS:C	2.56	0.43
1:B:417:GLN:O	1:B:418:GLY:C	2.55	0.43
1:B:201:ILE:CG2	1:B:258:THR:CG2	2.96	0.43
1:B:110:SER:CB	1:B:142:ARG:HH12	2.31	0.43
1:A:365:THR:HG22	1:A:366:MET:N	2.34	0.43
1:B:257:LYS:HB3	1:B:257:LYS:HE3	1.78	0.43
1:A:428:LYS:HD2	1:A:428:LYS:C	2.38	0.43
1:B:133:GLU:HA	1:B:431:ILE:HD11	2.00	0.43
1:A:132:ALA:O	1:A:133:GLU:C	2.54	0.43
1:B:95:LYS:HG3	1:B:95:LYS:HZ3	1.27	0.43
1:A:54:ASN:HB2	1:A:60:SER:OG	2.18	0.43
1:B:309:ASP:HB2	1:B:316:SER:HA	2.01	0.43
1:A:190:ARG:HD3	2:A:581:HOH:O	2.19	0.43
1:B:89:MET:CE	1:B:91:VAL:CG2	2.96	0.43
1:A:13:PRO:O	1:A:16:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:O	1:A:58:LYS:C	2.56	0.43
1:A:57:LEU:CD2	1:A:61:LEU:CD1	2.96	0.43
1:B:195:PRO:C	1:B:197:TYR:N	2.70	0.43
1:B:65:GLU:O	1:B:66:GLN:C	2.56	0.43
1:A:182:ASN:HA	1:A:281:LYS:O	2.18	0.43
1:A:179:ILE:HB	1:A:278:CYS:HB2	2.01	0.43
1:B:159:ILE:HG13	1:B:222:ILE:HD13	1.96	0.42
1:A:13:PRO:HA	1:A:16:ARG:HD3	2.00	0.42
1:B:163:LYS:O	1:B:167:SER:HB3	2.19	0.42
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.78	0.42
1:B:152:GLN:HB2	1:B:380:ASN:HB3	2.01	0.42
1:A:192:MET:SD	1:A:245:ASP:CB	2.97	0.42
1:A:286:VAL:HG13	1:A:292:ASN:CG	2.39	0.42
1:A:163:LYS:NZ	1:A:419:PHE:O	2.48	0.42
1:B:232:ALA:HA	1:B:264:LEU:O	2.19	0.42
1:A:245:ASP:C	1:A:248:GLY:N	2.73	0.42
1:A:26:THR:HG22	1:A:27:SER:HB3	2.00	0.42
1:A:110:SER:CB	1:A:142:ARG:HH22	2.32	0.42
1:B:85:LYS:HD3	2:B:494:HOH:O	2.19	0.42
1:B:101:GLU:O	1:B:102:VAL:C	2.57	0.42
1:B:278:CYS:SG	1:B:280:PHE:HD1	2.42	0.42
1:A:211:SER:O	1:A:212:PHE:C	2.56	0.42
1:B:183:GLY:HA3	1:B:207:LEU:HD12	2.02	0.42
1:B:53:TYR:CD2	1:B:53:TYR:O	2.73	0.42
1:B:284:THR:HA	1:B:285:PRO:C	2.40	0.42
1:B:301:LYS:CD	1:B:325:ILE:CD1	2.97	0.42
1:A:320:LEU:HB3	1:A:369:PHE:HB3	2.02	0.42
1:A:291:LYS:HA	1:A:291:LYS:HD3	1.69	0.42
1:B:375:ASN:OD1	1:B:375:ASN:C	2.58	0.42
1:B:87:ILE:HG21	1:B:90:ILE:HG12	2.01	0.41
1:A:251:THR:CG2	1:A:252:LYS:N	2.74	0.41
1:B:66:GLN:C	1:B:68:GLN:N	2.72	0.41
1:A:107:LEU:O	1:A:142:ARG:NH2	2.53	0.41
1:A:217:ASP:HB2	1:A:433:LEU:HD22	2.02	0.41
1:B:192:MET:SD	1:B:245:ASP:CB	3.02	0.41
1:A:428:LYS:HE2	1:A:432:ILE:HD11	2.03	0.41
1:B:79:GLU:HG3	1:B:109:HIS:CG	2.54	0.41
1:A:200:ASP:O	1:A:201:ILE:C	2.58	0.41
1:B:100:TYR:CZ	1:B:104:LYS:HD2	2.55	0.41
1:A:170:CYS:HB3	1:A:325:ILE:O	2.21	0.41
1:A:325:ILE:HD11	2:A:577:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:HG23	1:B:102:VAL:H	1.65	0.41
1:B:37:PHE:O	1:B:41:GLN:CB	2.68	0.41
1:B:179:ILE:HD13	1:B:179:ILE:HG21	1.83	0.41
1:A:208:ILE:H	1:A:208:ILE:HG13	1.62	0.41
1:A:446:GLU:O	1:A:447:GLU:HB2	2.20	0.41
1:B:293:LEU:HG	1:B:294:VAL:N	2.32	0.41
1:B:160:VAL:O	1:B:164:GLU:HG3	2.21	0.41
1:A:23:VAL:HG12	1:A:94:VAL:CG1	2.51	0.41
1:B:61:LEU:HA	1:B:61:LEU:HD12	1.62	0.41
1:A:2:ASN:O	1:A:10:SER:HA	2.21	0.41
1:A:113:ASN:OD1	1:A:113:ASN:C	2.59	0.41
1:B:78:LEU:O	1:B:81:PHE:HB3	2.21	0.41
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.77	0.40
1:B:192:MET:CE	1:B:245:ASP:O	2.69	0.40
1:B:192:MET:HE1	1:B:245:ASP:O	2.21	0.40
1:B:-6:TYR:CE2	1:B:394:LEU:HD11	2.56	0.40
1:B:0:LEU:HD23	1:B:0:LEU:HA	1.67	0.40
1:B:38:LEU:O	1:B:41:GLN:HB3	2.21	0.40
1:A:179:ILE:HD11	1:A:219:LEU:HD22	2.04	0.40
1:A:19:ARG:HG2	1:A:50:VAL:HG11	2.03	0.40
1:A:417:GLN:O	1:A:418:GLY:C	2.60	0.40
1:A:147:THR:HB	1:A:427:PHE:CD1	2.56	0.40
1:B:192:MET:HE1	1:B:245:ASP:HB2	2.01	0.40
1:B:58:LYS:O	1:B:61:LEU:N	2.54	0.40
1:A:57:LEU:HD23	1:A:61:LEU:HD13	2.01	0.40
1:B:48:GLN:HE21	1:B:71:HIS:CD2	2.39	0.40
1:B:53:TYR:CD2	1:B:53:TYR:C	2.89	0.40
1:A:75:PHE:HD2	1:A:80:SER:HB2	1.86	0.40

All (1) 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:76:ASP:OD2	2:B:601:HOH:O[3_556]	2.16	0.04

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	404/479 (84%)	386 (96%)	18 (4%)	0	100	100
1	B	393/479 (82%)	361 (92%)	30 (8%)	2 (0%)	34	30
All	All	797/958 (83%)	747 (94%)	48 (6%)	2 (0%)	46	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	SER
1	B	102	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/422 (88%)	318 (86%)	52 (14%)	4	2
1	B	359/422 (85%)	309 (86%)	50 (14%)	4	2
All	All	729/844 (86%)	627 (86%)	102 (14%)	4	2

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-9	GLU
1	A	5	LYS
1	A	7	SER
1	A	11	THR

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Mol	Chain	Res	Type
1	A	25	LEU
1	A	34	LYS
1	A	44	SER
1	A	48	GLN
1	A	56	THR
1	A	57	LEU
1	A	66	GLN
1	A	69	LEU
1	A	76	ASP
1	A	77	SER
1	A	80	SER
1	A	85	LYS
1	A	104	LYS
1	A	110	SER
1	A	111	SER
1	A	117	ARG
1	A	120	TYR
1	A	142	ARG
1	A	152	GLN
1	A	189	GLU
1	A	192	MET
1	A	193	ARG
1	A	196	GLU
1	A	201	ILE
1	A	203	SER
1	A	211	SER
1	A	240	THR
1	A	243	LEU
1	A	244	LEU
1	A	245	ASP
1	A	249	LYS
1	A	254	THR
1	A	256	SER
1	A	261	ASP
1	A	278	CYS
1	A	280	PHE
1	A	281	LYS
1	A	288	LYS
1	A	293	LEU
1	A	304	LEU
1	A	307	GLU
1	A	362	GLU

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Mol	Chain	Res	Type
1	A	366	MET
1	A	428	LYS
1	A	431	ILE
1	A	444	ASP
1	A	445	LYS
1	A	454	LYS
1	B	15	SER
1	B	29	LYS
1	B	48	GLN
1	B	56	THR
1	B	70	LYS
1	B	75	PHE
1	B	76	ASP
1	B	83	GLN
1	B	95	LYS
1	B	110	SER
1	B	111	SER
1	B	112	GLN
1	B	120	TYR
1	B	130	GLN
1	B	137	SER
1	B	139	SER
1	B	149	ILE
1	B	152	GLN
1	B	157	PRO
1	B	176	SER
1	B	194	SER
1	B	196	GLU
1	B	202	GLU
1	B	203	SER
1	B	211	SER
1	B	218	VAL
1	B	222	ILE
1	B	228	GLN
1	B	229	LYS
1	B	244	LEU
1	B	254	THR
1	B	256	SER
1	B	257	LYS
1	B	261	ASP
1	B	280	PHE
1	B	281	LYS

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Mol	Chain	Res	Type
1	B	287	LYS
1	B	316	SER
1	B	325	ILE
1	B	326	LYS
1	B	365	THR
1	B	366	MET
1	B	372	ARG
1	B	387	SER
1	B	415	ASP
1	B	428	LYS
1	B	431	ILE
1	B	435	ARG
1	B	453	SER
1	B	456	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-13	HIS
1	A	2	ASN
1	A	41	GLN
1	A	42	GLN
1	A	46	GLN
1	A	48	GLN
1	A	62	GLN
1	A	71	HIS
1	A	83	GLN
1	A	105	ASN
1	A	140	GLN
1	A	152	GLN
1	A	228	GLN
1	A	236	ASN
1	A	271	ASN
1	A	380	ASN
1	B	-13	HIS
1	B	42	GLN
1	B	66	GLN
1	B	71	HIS
1	B	83	GLN
1	B	112	GLN
1	B	115	ASN
1	B	152	GLN

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Mol	Chain	Res	Type
1	B	228	GLN
1	B	380	ASN

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 carbohydrates 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 ⓘ

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	413/479 (86%)	0.57	43 (10%) 8 12	19, 39, 81, 100	0
1	B	405/479 (84%)	0.67	41 (10%) 9 12	22, 41, 79, 100	0
All	All	818/958 (85%)	0.62	84 (10%) 9 12	19, 40, 81, 100	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	GLU	7.4
1	B	327	ASN	7.0
1	A	316	SER	6.3
1	B	328	GLY	6.2
1	B	245	ASP	5.8
1	A	192	MET	5.7
1	A	327	ASN	5.6
1	B	242	PHE	4.8
1	B	246	GLU	4.7
1	A	251	THR	4.2
1	B	193	ARG	4.1
1	B	244	LEU	4.0
1	A	328	GLY	3.9
1	A	363	GLU	3.9
1	B	61	LEU	3.8
1	A	61	LEU	3.8
1	A	244	LEU	3.8
1	A	252	LYS	3.7
1	B	251	THR	3.7
1	B	247	ASN	3.7
1	A	26	THR	3.7
1	B	362	GLU	3.6
1	A	7	SER	3.6
1	A	245	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	14	SER	3.4
1	B	259	CYS	3.4
1	A	9	LEU	3.3
1	A	250	ARG	3.3
1	A	242	PHE	3.2
1	A	115	ASN	3.1
1	B	254	THR	3.1
1	B	253	GLU	3.1
1	B	250	ARG	3.1
1	B	192	MET	3.0
1	A	3	ASN	3.0
1	B	252	LYS	3.0
1	A	12	VAL	2.9
1	B	316	SER	2.9
1	A	4	ASN	2.8
1	A	219	LEU	2.8
1	B	67	LEU	2.8
1	A	193	ARG	2.7
1	B	255	ILE	2.7
1	B	58	LYS	2.6
1	B	311	GLY	2.6
1	B	129	VAL	2.6
1	A	249	LYS	2.6
1	A	10	SER	2.5
1	B	64	ILE	2.5
1	A	5	LYS	2.4
1	B	115	ASN	2.4
1	A	6	ARG	2.3
1	A	62	GLN	2.3
1	B	323	TYR	2.3
1	B	243	LEU	2.3
1	A	218	VAL	2.3
1	A	56	THR	2.3
1	B	68	GLN	2.3
1	B	114	LEU	2.3
1	A	253	GLU	2.2
1	B	-11	SER	2.2
1	A	365	THR	2.2
1	B	256	SER	2.2
1	A	16	ARG	2.2
1	A	211	SER	2.2
1	A	216	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	65	GLU	2.2
1	A	362	GLU	2.2
1	B	196	GLU	2.2
1	A	151	LEU	2.1
1	A	278	CYS	2.1
1	B	136	TYR	2.1
1	A	326	LYS	2.1
1	B	65	GLU	2.1
1	A	294	VAL	2.1
1	B	325	ILE	2.1
1	B	142	ARG	2.1
1	A	57	LEU	2.1
1	A	212	PHE	2.1
1	A	179	ILE	2.1
1	B	264	LEU	2.1
1	A	309	ASP	2.1
1	B	31	TRP	2.0
1	B	202	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.