



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:09 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

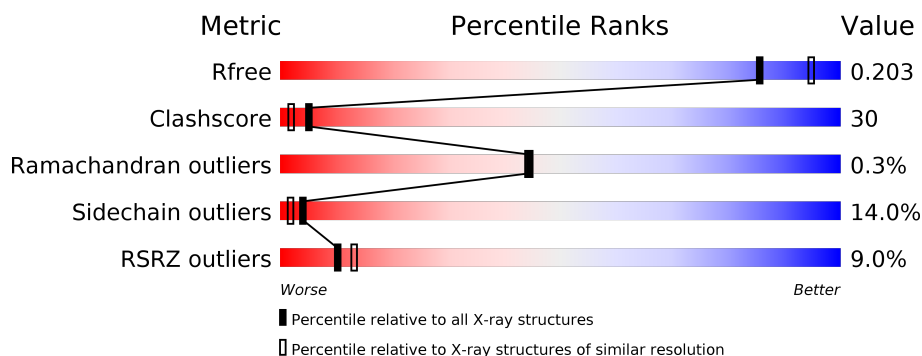
1 Overall quality at a glance

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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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>8%</div> <div>43% 35% 8% • 14%</div> </div>
1	B	479	<div> <div>8%</div> <div>39% 35% 10% • 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

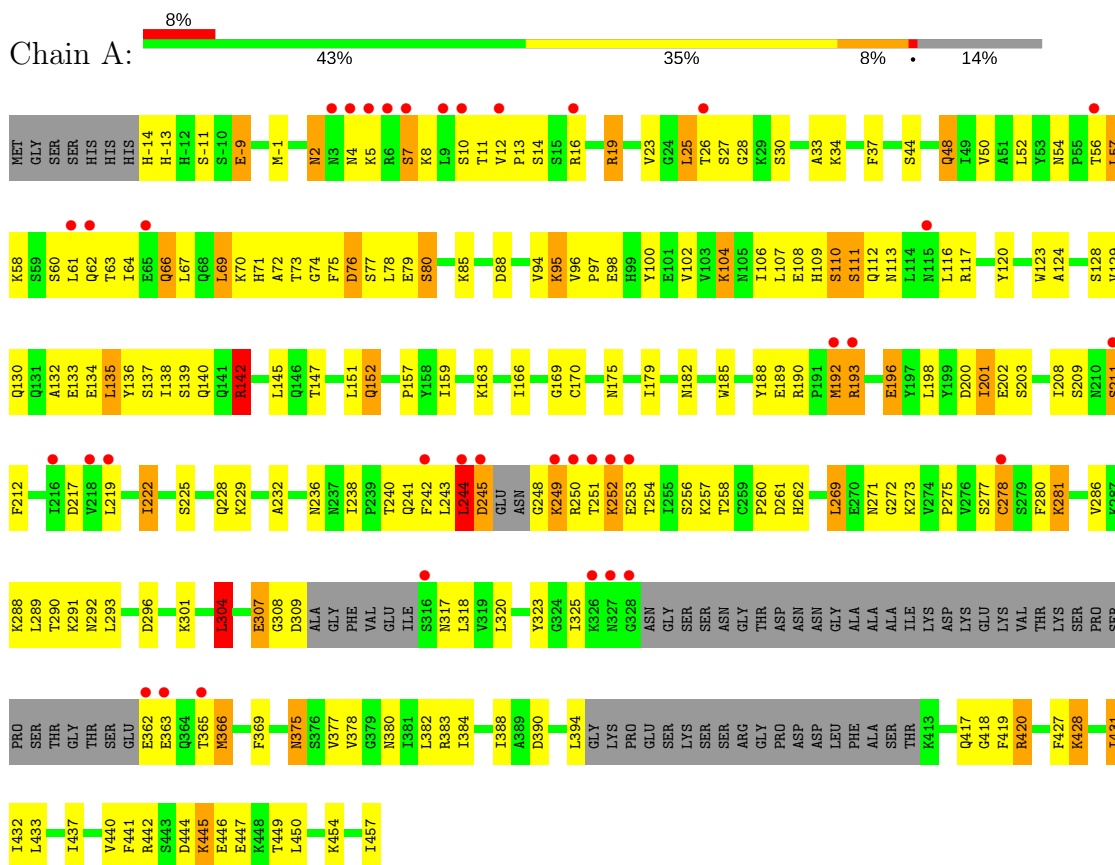
- Molecule 2 is water.

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

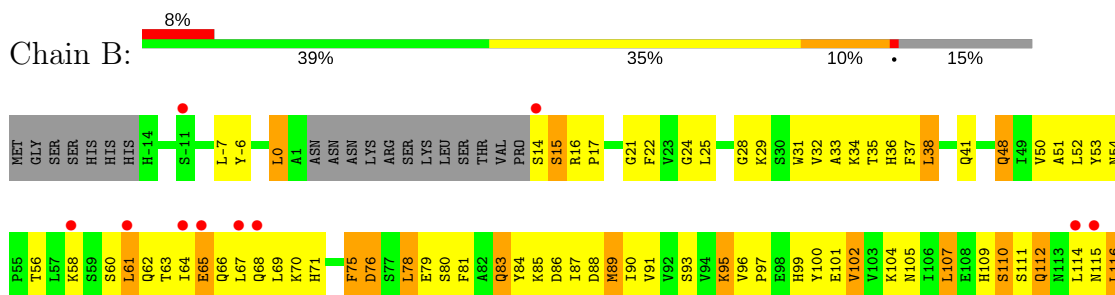
3 Residue-property plots

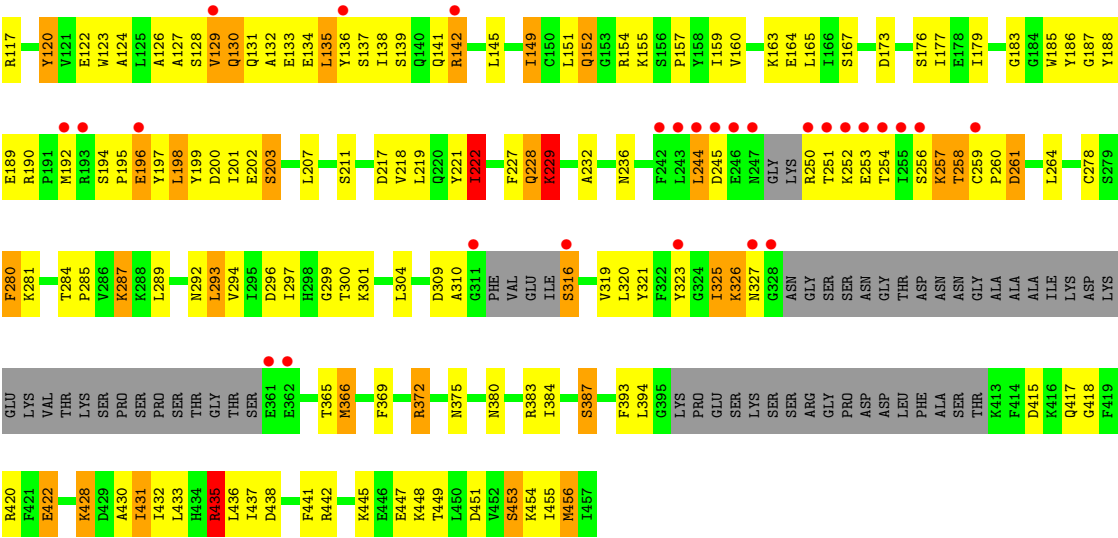
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Galactose/lactose metabolism regulatory protein GAL80



- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.20Å 137.10Å 72.90Å 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 2.08Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.195 , 0.245 0.199 , 0.203	Depositor DCC
R_{free} test set	6517 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 , 112.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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	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:H	1:B:152:GLN:HE21	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:201:ILE:HB	1:B:258:THR:HG22	1.68	0.75
1:B:428:LYS:O	1:B:428:LYS:HD2	1.87	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:A:67:LEU:HB2	1:A:69:LEU:HD21	1.72	0.72
1:B:257:LYS:HD2	1:B:259:CYS:O	1.90	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:A:12:VAL:HB	1:A:13:PRO:HD3	1.79	0.65
1:B:25:LEU:CD2	1:B:52:LEU:HD21	2.21	0.65
1:B:36:HIS:NE2	1:B:122:GLU:OE2	2.22	0.65
1:B:130:GLN:CD	1:B:130:GLN:H	1.98	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:A:269:LEU:O	1:A:273:LYS:HA	1.97	0.64
1:B:31:TRP:CZ2	1:B:35:THR:HG21	2.33	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:251:THR:HG22	1:B:253:GLU:N	2.11	0.63
1:B:435:ARG:HD2	1:B:455:ILE:O	1.97	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: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:80:SER:HA	1:B:83:GLN:NE2	2.15	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:A:79:GLU:HG3	1:A:109:HIS:CG	2.38	0.58
1:B:188:TYR:HD1	1:B:285:PRO:HD3	1.67	0.58
1:B:84:TYR:CZ	1:B:86:ASP:HB2	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:A:134:GLU:HA	1:A:137:SER:OG	2.05	0.56
1:B:123:TRP:CG	1:B:124:ALA:HA	2.39	0.56
1:B:250:ARG:HG2	1:B:251:THR:N	2.20	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:A:236:ASN:ND2	1:A:260:PRO:HA	2.20	0.56
1:B:31:TRP:CE2	1:B:35:THR:HG21	2.41	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: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:25:LEU:HD13	1:B:32:VAL:HG12	1.89	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:13:PRO:HA	1:A:16:ARG:NH1	2.22	0.55
1:A:62:GLN:O	1:A:66:GLN:HG3	2.06	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:C	1:A:304:LEU:HD23	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:24:GLY:HA3	1:B:93:SER:O	2.07	0.54
2:A:512:HOH:O	1:B:287:LYS:HG2	2.08	0.54
1:B:384:ILE:O	1:B:387:SER:HB2	2.08	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:-13:HIS:O	1:A:-13:HIS:HD2	1.90	0.53
1:A:12:VAL:CB	1:A:13:PRO:HD3	2.37	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:A:262:HIS:CE1	1:A:281:LYS:HG3	2.44	0.52
1:B:14:SER:O	1:B:16:ARG:N	2.42	0.52
1:A:128:SER:HB2	1:A:130:GLN:OE1	2.09	0.52
1:B:201:ILE:CG2	1:B:258:THR:HG22	2.40	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:A:100:TYR:O	1:A:104:LYS:HB2	2.09	0.51
1:B:163:LYS:HE3	1:B:221:TYR:CE2	2.46	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:A:102:VAL:HG12	1:A:106:ILE:HD12	1.92	0.51
1:B:128:SER:HG	1:B:130:GLN:HG2	1.76	0.51
1:A:79:GLU:HG3	1:A:109:HIS:CD2	2.46	0.50
1:A:251:THR:HG21	1:A:253:GLU:CB	2.41	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:A:134:GLU:O	1:A:137:SER:OG	2.27	0.50
1:B:431:ILE:O	1:B:435:ARG:CG	2.59	0.50
1:A:157:PRO:HG3	1:A:383:ARG:NH1	2.27	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:B:455:ILE:CG1	1:B:456:MET:HE3	2.42	0.50
1:A:70:LYS:HE3	1:A:71:HIS:NE2	2.27	0.50
1:A:8:LYS:O	1:A:14:SER:OG	2.27	0.50
1:B:34:LYS:O	1:B:38:LEU:HD12	2.12	0.50
1:B:325:ILE:C	1:B:327:ASN:H	2.15	0.50
1:B:35:THR:OG1	1:B:36:HIS:N	2.39	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:323:TYR:HA	1:A:365:THR:O	2.12	0.49
1:A:63:THR:HA	1:A:66:GLN:OE1	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: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:B:200:ASP:O	1:B:203:SER:OG	2.28	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:120:TYR:C	1:B:120:TYR:HD2	2.16	0.48
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:A:57:LEU:CD2	1:A:61:LEU:HD11	2.44	0.48
1:B:96:VAL:N	1:B:97:PRO:HD3	2.27	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:260:PRO:HD2	2:A:498:HOH:O	2.14	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: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:227:PHE:HB2	2:B:535:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HG21	1:B:438:ASP:OD1	2.14	0.48
1:A:175:ASN:O	1:A:275:PRO:HD2	2.14	0.48
1:A:232:ALA:CB	1:A:440:VAL:HG13	2.44	0.48
1:A:94:VAL:O	1:A:95:LYS:C	2.51	0.48
1:A:107:LEU:HD13	1:A:138:ILE:CG2	2.43	0.48
1:A:4:ASN:O	1:A:7:SER:HB3	2.14	0.48
1:B:112:GLN:HG2	2:B:581:HOH:O	2.14	0.48
1:B:188:TYR:CD1	1:B:285:PRO:HD3	2.48	0.48
1:A:96:VAL:N	1:A:97:PRO:CD	2.76	0.47
1:A:139:SER:O	1:A:140:GLN:C	2.51	0.47
1:B:128:SER:CB	1:B:130:GLN:HG2	2.44	0.47
1:B:120:TYR:C	1:B:120:TYR:CD2	2.87	0.47
1:B:244:LEU:CD2	1:B:250:ARG:HG3	2.45	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: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:B:177:ILE:HG12	1:B:297:ILE:HG12	1.97	0.46
1:B:95:LYS:C	1:B:97:PRO:HD2	2.35	0.46
1:A:225:SER:HB2	1:A:271:ASN:ND2	2.31	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:B:441:PHE:O	1:B:445:LYS:CG	2.61	0.46
1:B:135:LEU:HA	1:B:135:LEU:HD23	1.67	0.46
1:B:96:VAL:HA	1:B:99:HIS:CD2	2.51	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:HA	1:A:193:ARG:HD2	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:A:25:LEU:C	1:A:25:LEU:HD12	2.29	0.45
1:B:14:SER:C	1:B:16:ARG:N	2.69	0.45
1:B:152:GLN:CA	1:B:384:ILE:HD11	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD23	1:A:61:LEU:HD11	1.97	0.45
1:B:130:GLN:N	1:B:130:GLN:CD	2.67	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:-13:HIS:O	1:A:-13:HIS:CD2	2.70	0.45
1:A:289:LEU:HD21	1:B:323:TYR:HB2	1.98	0.45
1:A:229:LYS:HD2	1:A:449:THR:HG21	1.99	0.45
1:B:201:ILE:HG22	1:B:258:THR:HG21	1.99	0.44
1:B:136:TYR:CG	1:B:431:ILE:HD13	2.52	0.44
1:B:62:GLN:C	1:B:66:GLN:HE21	2.20	0.44
1:A:166:ILE:HD12	1:A:222:ILE:HG22	1.98	0.44
1:A:244:LEU:HA	1:A:249:LYS:O	2.18	0.44
1:A:441:PHE:O	1:A:445:LYS:N	2.47	0.44
1:A:229:LYS:HA	1:A:450:LEU:O	2.18	0.44
1:A:377:VAL:CG1	1:A:378:VAL:HG23	2.48	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:A:365:THR:HG22	1:A:366:MET:N	2.34	0.43
1:B:110:SER:CB	1:B:142:ARG:HH12	2.31	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:A:132:ALA:O	1:A:133:GLU:C	2.54	0.43
1:A:190:ARG:HD3	2:A:581:HOH:O	2.19	0.43
1:A:54:ASN:HB2	1:A:60:SER:OG	2.18	0.43
1:B:133:GLU:HA	1:B:431:ILE:HD11	2.00	0.43
1:B:309:ASP:HB2	1:B:316:SER:HA	2.01	0.43
1:B:95:LYS:HG3	1:B:95:LYS:HZ3	1.27	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: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: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:B:159:ILE:HG13	1:B:222:ILE:HD13	1.96	0.42
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.78	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: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:B:152:GLN:HB2	1:B:380:ASN:HB3	2.01	0.42
1:A:110:SER:CB	1:A:142:ARG:HH22	2.32	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: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:A:211:SER:O	1:A:212:PHE:C	2.56	0.42
1:B:278:CYS:SG	1:B:280:PHE:HD1	2.42	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:A:291:LYS:HA	1:A:291:LYS:HD3	1.69	0.42
1:A:320:LEU:HB3	1:A:369:PHE:HB3	2.02	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: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:200:ASP:O	1:A:201:ILE:C	2.58	0.41
1:A:428:LYS:HE2	1:A:432:ILE:HD11	2.03	0.41
1:B:100:TYR:CZ	1:B:104:LYS:HD2	2.55	0.41
1:B:79:GLU:HG3	1:B:109:HIS:CG	2.54	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: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:179:ILE:HD13	1:B:179:ILE:HG21	1.83	0.41
1:B:37:PHE:O	1:B:41:GLN:CB	2.68	0.41
1:B:160:VAL:O	1:B:164:GLU:HG3	2.21	0.41
1:B:293:LEU:HG	1:B:294:VAL:N	2.32	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: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: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:0:LEU:HD23	1:B:0:LEU:HA	1.67	0.40
1:B:192:MET:HE1	1:B:245:ASP:O	2.21	0.40
1:B:192:MET:CE	1:B:245:ASP:O	2.69	0.40
1:B:-6:TYR:CE2	1:B:394:LEU:HD11	2.56	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:B:38:LEU:O	1:B:41:GLN:HB3	2.21	0.40
1:A:147:THR:HB	1:A:427:PHE:CD1	2.56	0.40
1:A:417:GLN:O	1:A:418:GLY:C	2.60	0.40
1:A:57:LEU:HD23	1:A:61:LEU:HD13	2.01	0.40
1:A:75:PHE:HD2	1:A:80:SER:HB2	1.86	0.40
1:B:192:MET:HE1	1:B:245:ASP:HB2	2.01	0.40
1:B:53:TYR:CD2	1:B:53:TYR:C	2.89	0.40
1:B:58:LYS:O	1:B:61:LEU:N	2.54	0.40
1:B:48:GLN:HE21	1:B:71:HIS:CD2	2.39	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%)	32	28
All	All	797/958 (83%)	747 (94%)	48 (6%)	2 (0%)	44	44

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%)	0.50	37 (8%) 10 13	19, 39, 81, 100	0
1	B	405/479 (84%)	0.59	37 (9%) 10 13	22, 41, 79, 100	0
All	All	818/958 (85%)	0.54	74 (9%) 10 13	19, 40, 81, 100	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	GLU	7.2
1	B	327	ASN	6.8
1	A	316	SER	6.0
1	B	328	GLY	5.9
1	B	245	ASP	5.6
1	A	192	MET	5.5
1	A	327	ASN	5.5
1	B	246	GLU	4.6
1	B	242	PHE	4.6
1	A	251	THR	4.0
1	B	193	ARG	4.0
1	B	244	LEU	3.8
1	A	328	GLY	3.8
1	A	363	GLU	3.7
1	B	61	LEU	3.6
1	A	61	LEU	3.6
1	A	244	LEU	3.6
1	A	252	LYS	3.6
1	B	247	ASN	3.6
1	B	251	THR	3.5
1	B	362	GLU	3.5
1	A	26	THR	3.5
1	A	7	SER	3.4
1	A	245	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	14	SER	3.3
1	A	250	ARG	3.2
1	B	259	CYS	3.2
1	A	9	LEU	3.1
1	A	115	ASN	3.0
1	B	253	GLU	3.0
1	A	242	PHE	3.0
1	B	250	ARG	3.0
1	B	254	THR	3.0
1	B	192	MET	2.9
1	A	3	ASN	2.9
1	B	252	LYS	2.9
1	B	316	SER	2.8
1	A	12	VAL	2.7
1	A	4	ASN	2.7
1	A	219	LEU	2.6
1	A	193	ARG	2.6
1	B	67	LEU	2.6
1	B	58	LYS	2.5
1	B	255	ILE	2.5
1	A	249	LYS	2.5
1	B	311	GLY	2.5
1	A	10	SER	2.4
1	B	129	VAL	2.4
1	A	5	LYS	2.3
1	B	64	ILE	2.3
1	B	115	ASN	2.3
1	A	6	ARG	2.2
1	A	62	GLN	2.2
1	B	323	TYR	2.2
1	B	68	GLN	2.2
1	A	253	GLU	2.2
1	B	243	LEU	2.1
1	A	56	THR	2.1
1	B	-11	SER	2.1
1	A	16	ARG	2.1
1	A	65	GLU	2.1
1	B	114	LEU	2.1
1	B	256	SER	2.1
1	A	218	VAL	2.1
1	A	365	THR	2.1
1	A	362	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	196	GLU	2.1
1	A	211	SER	2.1
1	B	136	TYR	2.0
1	A	326	LYS	2.0
1	A	278	CYS	2.0
1	B	65	GLU	2.0
1	A	216	ILE	2.0
1	B	142	ARG	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.