



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:53 AM EDT

PDB ID : 1PXT / pdb_00001pxt
Title : THE 2.8 ANGSTROMS STRUCTURE OF PEROXISOMAL 3-KETOACYL-COA THIOLASE OF SACCHAROMYCES CEREVISIAE: A FIVE LAYERED A-B-A-B-A STRUCTURE, CONSTRUCTED FROM TWO CORE DOMAINS OF IDENTICAL TOPOLOGY
Authors : Mathieu, M.; Wierenga, R.K.
Deposited on : 1994-07-04
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

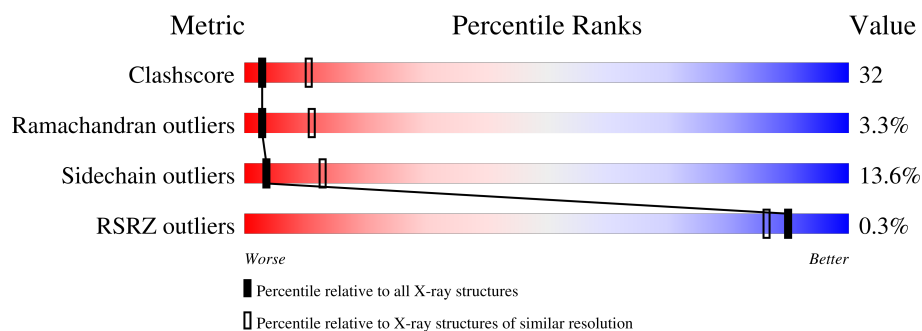
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	390	
1	B	390	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5201 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.

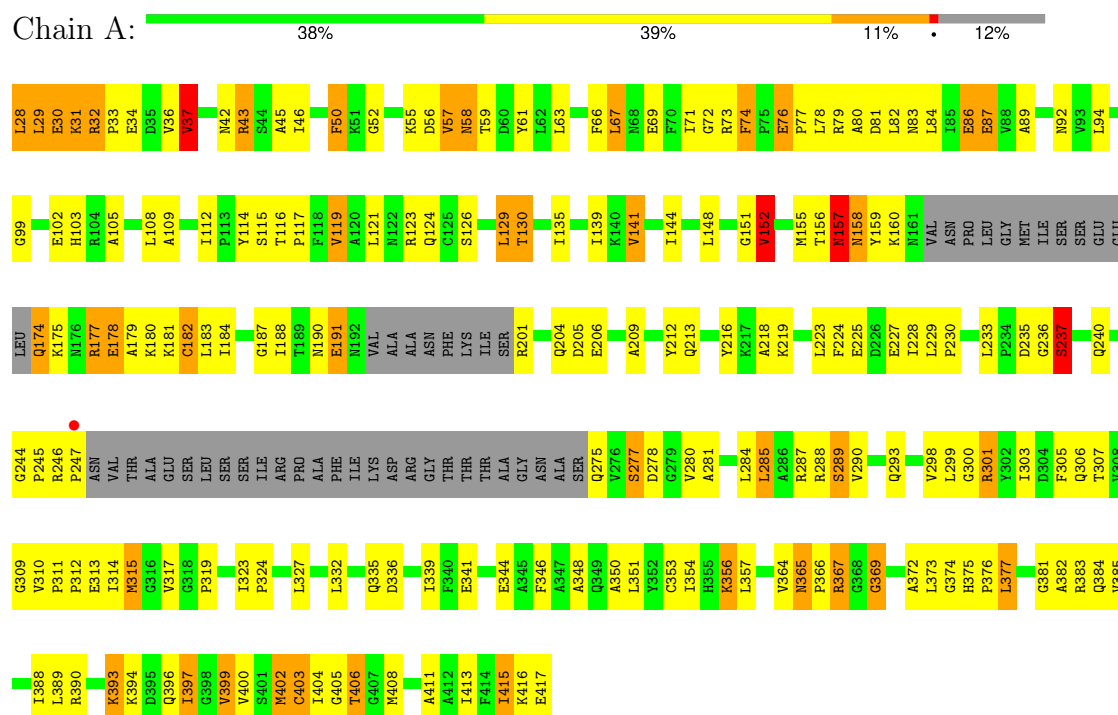
- Molecule 1 is a protein called PEROXISOMAL 3-KETOACYL-COA THIOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2585	1634	452	486	13			
1	B	348	Total	C	N	O	S	0	0	0
			2616	1651	457	495	13			

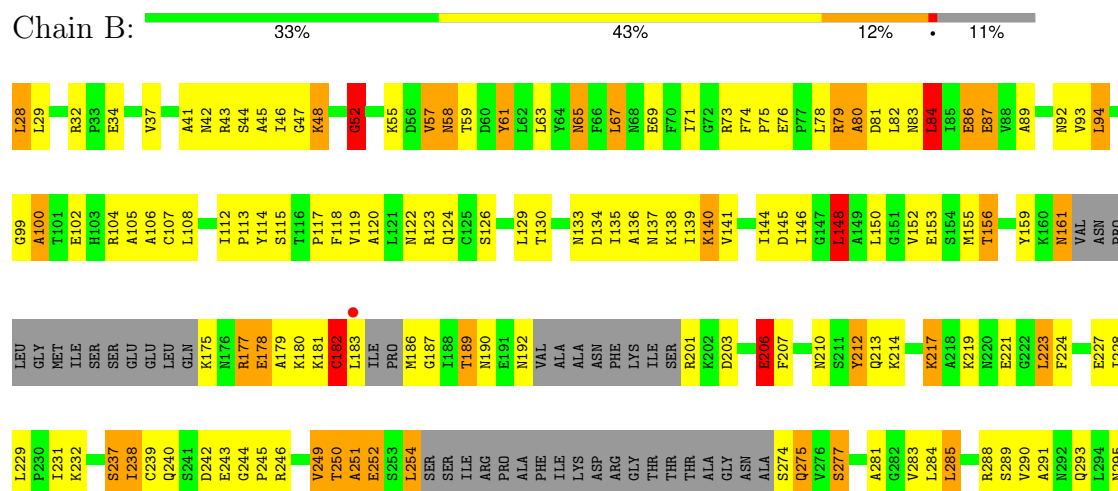
3 Residue-property plots

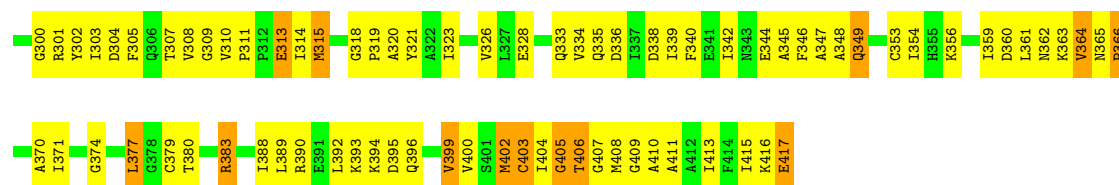
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PEROXISOMAL 3-KETOACYL-COA THIOLASE



• Molecule 1: PEROXISOMAL 3-KETOACYL-COA THIOLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.78Å 93.72Å 120.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 88.5 (8.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.75Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , 0.334 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 139.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5201	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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	0.80	1/2622 (0.0%)	1.25	28/3543 (0.8%)
1	B	0.85	1/2651 (0.0%)	1.31	35/3581 (1.0%)
All	All	0.83	2/5273 (0.0%)	1.28	63/7124 (0.9%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	ILE	CA-CB	5.59	1.61	1.54
1	B	140	LYS	CA-C	-5.25	1.46	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	345	ALA	N-CA-C	-8.73	101.71	111.14
1	B	84	LEU	N-CA-C	-7.96	103.59	113.38
1	A	30	GLU	N-CA-C	-7.46	98.09	109.95
1	A	45	ALA	N-CA-C	-7.32	98.63	110.20
1	A	152	VAL	CB-CA-C	-7.23	100.67	111.80
1	A	237	SER	N-CA-C	7.09	120.43	108.23
1	B	318	GLY	CA-C-N	6.79	127.35	119.47
1	B	318	GLY	C-N-CA	6.79	127.35	119.47
1	B	100	ALA	N-CA-C	6.74	119.48	111.33
1	B	76	GLU	CA-C-N	-6.71	111.89	119.28
1	B	76	GLU	C-N-CA	-6.71	111.89	119.28
1	B	380	THR	N-CA-C	6.67	119.11	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	N-CA-C	-6.49	104.12	111.07
1	A	191	GLU	N-CA-C	-6.44	104.35	111.82
1	B	223	LEU	N-CA-C	6.43	119.98	111.75
1	B	217	LYS	N-CA-C	-6.23	104.18	110.97
1	A	369	GLY	N-CA-C	6.22	119.84	111.20
1	A	327	LEU	N-CA-C	-6.16	104.20	111.03
1	B	189	THR	N-CA-C	-6.09	105.11	112.54
1	A	158	ASN	N-CA-C	6.00	120.60	113.16
1	B	238	ILE	N-CA-C	-6.00	100.43	108.35
1	A	37	VAL	N-CA-C	5.99	116.56	108.17
1	A	403	CYS	N-CA-C	-5.91	102.57	110.55
1	A	365	ASN	CA-C-N	5.89	127.20	119.84
1	A	365	ASN	C-N-CA	5.89	127.20	119.84
1	A	364	VAL	N-CA-C	5.85	117.19	108.23
1	B	249	VAL	N-CA-C	-5.85	101.11	108.84
1	B	206	GLU	N-CA-C	-5.85	104.81	111.07
1	B	107	CYS	N-CA-C	-5.83	104.83	111.07
1	B	403	CYS	N-CA-C	-5.82	101.87	110.48
1	B	364	VAL	N-CA-C	5.77	116.61	108.36
1	A	112	ILE	N-CA-C	-5.72	103.34	108.95
1	B	148	LEU	N-CA-C	5.67	117.97	108.96
1	B	239	CYS	N-CA-C	5.66	118.77	107.62
1	B	395	ASP	N-CA-C	5.66	119.48	112.24
1	B	65	ASN	N-CA-C	5.63	117.09	111.07
1	B	182	CYS	N-CA-C	5.63	122.78	110.80
1	B	52	GLY	N-CA-C	5.58	126.41	113.18
1	A	119	VAL	CB-CA-C	-5.56	101.49	110.28
1	A	94	LEU	N-CA-C	5.55	120.94	113.72
1	B	275	GLN	N-CA-C	5.53	118.48	109.24
1	A	301	ARG	N-CA-C	5.51	117.64	108.99
1	B	250	THR	N-CA-C	5.49	119.48	112.12
1	A	225	GLU	N-CA-C	5.49	118.09	111.40
1	A	182	CYS	N-CA-C	-5.48	106.47	112.72
1	A	89	ALA	N-CA-C	-5.48	100.75	109.96
1	A	373	LEU	N-CA-C	5.47	118.17	111.82
1	B	93	VAL	N-CA-C	5.40	118.36	112.96
1	A	336	ASP	N-CA-C	-5.38	106.40	113.17
1	B	112	ILE	CA-C-N	5.36	125.35	119.89
1	B	112	ILE	C-N-CA	5.36	125.35	119.89
1	A	37	VAL	N-CA-CB	-5.35	103.97	111.25
1	A	157	ASN	N-CA-C	5.33	117.90	111.40
1	B	61	TYR	N-CA-C	-5.24	105.25	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ALA	N-CA-C	-5.21	102.57	110.28
1	B	336	ASP	N-CA-C	-5.21	106.61	113.17
1	B	94	LEU	N-CA-C	5.20	120.48	113.72
1	A	377	LEU	N-CA-C	5.19	121.85	110.80
1	A	151	GLY	N-CA-C	-5.15	100.97	113.18
1	B	227	GLU	N-CA-C	5.10	118.77	112.54
1	A	52	GLY	N-CA-C	5.09	119.08	112.25
1	B	399	VAL	CB-CA-C	-5.04	102.84	110.95
1	B	80	ALA	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	321	TYR	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	2585	0	2628	165	0
1	B	2616	0	2655	187	0
All	All	5201	0	5283	339	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 32.

All (339) 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:28:LEU:HD21	1:A:332:LEU:HD21	1.27	1.06
1:A:50:PHE:H	1:A:156:THR:HG22	1.20	1.00
1:A:28:LEU:HD11	1:A:332:LEU:HD11	1.47	0.94
1:B:81:ASP:HB3	1:B:84:LEU:HD12	1.45	0.94
1:B:63:LEU:HD11	1:B:150:LEU:HD13	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:HD3	1:A:130:THR:HG21	1.50	0.91
1:A:288:ARG:HH21	1:A:301:ARG:HD3	1.35	0.90
1:A:123:ARG:CD	1:A:130:THR:HG21	2.07	0.84
1:B:275:GLN:HB2	1:B:374:GLY:HA2	1.59	0.84
1:A:50:PHE:N	1:A:156:THR:HG22	1.92	0.84
1:A:175:LYS:HA	1:A:180:LYS:HE3	1.59	0.83
1:A:288:ARG:NH2	1:A:301:ARG:HD3	1.95	0.81
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.45	0.81
1:A:117:PRO:HB2	1:B:123:ARG:HH21	1.49	0.78
1:A:117:PRO:HB2	1:B:123:ARG:NH2	2.00	0.77
1:B:41:ALA:H	1:B:73:ARG:HH12	1.32	0.76
1:B:244:GLY:H	1:B:245:PRO:HD2	1.51	0.75
1:B:354:ILE:HD11	1:B:364:VAL:HG11	1.67	0.75
1:A:300:GLY:HA2	1:A:417:GLU:H	1.53	0.74
1:B:63:LEU:HD23	1:B:106:ALA:HB3	1.68	0.74
1:A:416:LYS:O	1:A:417:GLU:HB2	1.86	0.74
1:B:177:ARG:H	1:B:180:LYS:HE3	1.50	0.74
1:A:341:GLU:HB2	1:A:388:ILE:HD12	1.70	0.73
1:A:37:VAL:HG13	1:A:298:VAL:HG13	1.69	0.73
1:B:300:GLY:HA2	1:B:417:GLU:H	1.53	0.73
1:B:404:ILE:HB	1:B:408:MET:HB2	1.69	0.73
1:B:126:SER:HA	1:B:402:MET:HE2	1.71	0.73
1:A:71:ILE:O	1:A:74:PHE:HB2	1.88	0.72
1:B:136:ALA:O	1:B:140:LYS:HG3	1.89	0.72
1:A:309:GLY:HA3	1:B:114:TYR:O	1.91	0.71
1:B:123:ARG:HD3	1:B:130:THR:HG21	1.71	0.70
1:A:105:ALA:HB1	1:B:179:ALA:HB1	1.73	0.70
1:B:74:PHE:O	1:B:79:ARG:HD3	1.91	0.70
1:B:206:GLU:HG2	1:B:207:PHE:N	2.06	0.70
1:A:404:ILE:HB	1:A:408:MET:HB2	1.72	0.70
1:A:275:GLN:HB2	1:A:374:GLY:HA2	1.72	0.70
1:B:58:ASN:HD22	1:B:59:THR:H	1.40	0.69
1:A:123:ARG:HH21	1:B:117:PRO:HB2	1.57	0.69
1:B:55:LYS:HA	1:B:156:THR:HG21	1.73	0.69
1:A:175:LYS:HA	1:A:180:LYS:CE	2.22	0.69
1:B:189:THR:HA	1:B:192:ASN:HD22	1.56	0.69
1:A:141:VAL:HG11	1:B:137:ASN:OD1	1.92	0.68
1:B:189:THR:HA	1:B:192:ASN:ND2	2.08	0.68
1:A:28:LEU:HD21	1:A:332:LEU:CD2	2.15	0.67
1:A:152:VAL:HG13	1:A:280:VAL:HG22	1.76	0.67
1:B:274:SER:HA	1:B:371:ILE:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:HD23	1:B:415:ILE:HD13	1.77	0.66
1:B:416:LYS:O	1:B:417:GLU:HB2	1.96	0.66
1:A:175:LYS:HG2	1:A:180:LYS:NZ	2.11	0.65
1:B:86:GLU:HG3	1:B:144:ILE:HB	1.77	0.65
1:A:246:ARG:O	1:A:246:ARG:HG3	1.98	0.64
1:B:251:ALA:O	1:B:252:GLU:HG3	1.97	0.64
1:A:155:MET:HE3	1:A:277:SER:H	1.61	0.64
1:B:42:ASN:HD22	1:B:229:LEU:HD11	1.63	0.64
1:B:63:LEU:HD11	1:B:150:LEU:CD1	2.27	0.64
1:A:28:LEU:CD1	1:A:332:LEU:HD11	2.26	0.63
1:A:301:ARG:HH21	1:A:415:ILE:HD12	1.62	0.63
1:B:311:PRO:HB2	1:B:314:ILE:HG12	1.80	0.63
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.63	0.63
1:A:92:ASN:ND2	1:A:103:HIS:HE1	1.97	0.63
1:B:123:ARG:CD	1:B:130:THR:HG21	2.29	0.62
1:B:100:ALA:HB2	1:B:120:ALA:HB2	1.79	0.62
1:B:346:PHE:O	1:B:349:GLN:HG3	2.00	0.62
1:B:354:ILE:CD1	1:B:364:VAL:HG11	2.29	0.62
1:A:63:LEU:HG	1:A:67:LEU:CD2	2.30	0.62
1:A:397:ILE:HG12	1:A:415:ILE:HG12	1.83	0.61
1:B:44:SER:HB2	1:B:231:ILE:HD12	1.81	0.61
1:B:190:ASN:HD21	1:B:348:ALA:HB3	1.66	0.61
1:B:187:GLY:O	1:B:190:ASN:HB3	2.01	0.61
1:A:123:ARG:HD3	1:A:130:THR:CG2	2.29	0.61
1:A:344:GLU:CD	1:A:369:GLY:HA3	2.26	0.61
1:B:41:ALA:N	1:B:73:ARG:HH12	1.97	0.60
1:A:339:ILE:HD12	1:A:366:PRO:HG2	1.83	0.60
1:A:86:GLU:O	1:A:87:GLU:HB2	2.01	0.60
1:A:33:PRO:O	1:A:288:ARG:HB3	2.02	0.60
1:A:344:GLU:OE2	1:A:369:GLY:HA3	2.02	0.59
1:B:246:ARG:NH1	1:B:249:VAL:HG22	2.18	0.59
1:A:389:LEU:O	1:A:416:LYS:HE2	2.02	0.59
1:B:320:ALA:HB1	1:B:356:LYS:HD2	1.84	0.59
1:B:71:ILE:O	1:B:74:PHE:HB2	2.02	0.59
1:A:123:ARG:CZ	1:B:119:VAL:HG22	2.33	0.59
1:A:50:PHE:H	1:A:156:THR:CG2	2.05	0.59
1:A:218:ALA:CB	1:A:223:LEU:HD12	2.33	0.58
1:B:340:PHE:CE2	1:B:359:ILE:HG23	2.39	0.58
1:A:216:TYR:HB2	1:A:247:PRO:HD2	1.85	0.58
1:A:144:ILE:O	1:A:287:ARG:NH2	2.36	0.58
1:B:43:ARG:NH2	1:B:228:ILE:HD11	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASN:O	1:B:214:LYS:HG3	2.03	0.58
1:A:141:VAL:O	1:A:141:VAL:HG13	2.04	0.58
1:A:218:ALA:HB1	1:A:223:LEU:HD12	1.86	0.57
1:A:78:LEU:HD13	1:A:284:LEU:HD21	1.86	0.57
1:B:42:ASN:ND2	1:B:229:LEU:HD21	2.19	0.57
1:B:177:ARG:O	1:B:179:ALA:N	2.38	0.57
1:B:237:SER:O	1:B:238:ILE:HG13	2.04	0.57
1:A:190:ASN:HD21	1:A:348:ALA:HB3	1.70	0.57
1:B:360:ASP:OD1	1:B:362:ASN:HB2	2.05	0.57
1:A:179:ALA:HB1	1:B:105:ALA:HB1	1.86	0.56
1:B:177:ARG:HG2	1:B:178:GLU:H	1.70	0.56
1:B:400:VAL:O	1:B:411:ALA:HA	2.04	0.56
1:A:81:ASP:C	1:A:83:ASN:H	2.13	0.56
1:B:246:ARG:HG3	1:B:246:ARG:NH1	2.19	0.56
1:A:135:ILE:O	1:A:139:ILE:HG13	2.05	0.56
1:A:233:LEU:HD12	1:A:237:SER:O	2.05	0.56
1:A:305:PHE:O	1:A:306:GLN:HG2	2.05	0.56
1:B:219:LYS:HD2	1:B:245:PRO:HG2	1.88	0.56
1:A:126:SER:HA	1:A:402:MET:HE2	1.88	0.55
1:B:81:ASP:HB3	1:B:84:LEU:CD1	2.29	0.55
1:B:393:LYS:O	1:B:396:GLN:HG3	2.06	0.55
1:B:83:ASN:HB3	1:B:113:PRO:HG3	1.88	0.55
1:A:365:ASN:N	1:A:366:PRO:HD3	2.21	0.55
1:B:389:LEU:O	1:B:416:LYS:HE2	2.05	0.55
1:A:188:ILE:O	1:A:191:GLU:HB2	2.06	0.55
1:A:201:ARG:HA	1:A:204:GLN:HG3	1.89	0.55
1:B:177:ARG:N	1:B:180:LYS:HE3	2.21	0.55
1:B:288:ARG:HG3	1:B:288:ARG:HH11	1.72	0.55
1:B:82:LEU:C	1:B:84:LEU:H	2.15	0.55
1:A:129:LEU:HD12	1:A:402:MET:SD	2.48	0.54
1:A:175:LYS:HG2	1:A:180:LYS:HZ1	1.72	0.54
1:A:280:VAL:HG12	1:A:281:ALA:N	2.22	0.54
1:A:356:LYS:HE3	1:A:356:LYS:HA	1.88	0.54
1:B:126:SER:HA	1:B:402:MET:CE	2.37	0.54
1:A:155:MET:O	1:A:159:TYR:HB2	2.07	0.54
1:A:323:ILE:HB	1:A:357:LEU:HD11	1.88	0.54
1:B:44:SER:CB	1:B:231:ILE:HD12	2.37	0.54
1:A:92:ASN:HD22	1:A:103:HIS:CE1	2.26	0.53
1:A:123:ARG:NH2	1:B:117:PRO:HB2	2.22	0.53
1:A:230:PRO:HA	1:A:240:GLN:HB3	1.89	0.53
1:B:29:LEU:CD2	1:B:415:ILE:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:O	1:B:370:ALA:HB3	2.07	0.53
1:B:92:ASN:O	1:B:122:ASN:HB2	2.08	0.53
1:A:281:ALA:HB3	1:A:382:ALA:HB3	1.90	0.53
1:B:48:LYS:O	1:B:52:GLY:HA3	2.09	0.53
1:B:86:GLU:O	1:B:87:GLU:HB2	2.09	0.53
1:A:31:LYS:O	1:A:31:LYS:HD3	2.09	0.53
1:A:141:VAL:O	1:A:141:VAL:CG1	2.57	0.52
1:B:69:GLU:HB3	1:B:229:LEU:HD13	1.90	0.52
1:B:118:PHE:CD1	1:B:118:PHE:C	2.87	0.52
1:A:36:VAL:HG12	1:A:285:LEU:HD12	1.90	0.52
1:A:209:ALA:O	1:A:213:GLN:HG3	2.09	0.52
1:A:367:ARG:HH11	1:A:367:ARG:CG	2.22	0.52
1:B:213:GLN:O	1:B:217:LYS:HG3	2.09	0.52
1:B:289:SER:O	1:B:293:GLN:HG3	2.10	0.52
1:A:43:ARG:NH1	1:A:227:GLU:OE2	2.42	0.52
1:A:174:GLN:OE1	1:A:175:LYS:HG3	2.10	0.52
1:B:145:ASP:HB3	1:B:290:VAL:HG21	1.92	0.52
1:B:365:ASN:N	1:B:366:PRO:HD3	2.25	0.52
1:A:32:ARG:H	1:A:32:ARG:HE	1.56	0.51
1:B:232:LYS:HG3	1:B:238:ILE:HG12	1.91	0.51
1:A:92:ASN:HD22	1:A:103:HIS:HE1	1.59	0.51
1:B:63:LEU:HG	1:B:67:LEU:HD22	1.92	0.51
1:B:338:ASP:O	1:B:339:ILE:HD13	2.10	0.51
1:B:315:MET:HE2	1:B:403:CYS:SG	2.50	0.51
1:B:81:ASP:O	1:B:84:LEU:HB2	2.11	0.51
1:A:155:MET:HE2	1:A:376:PRO:HA	1.92	0.51
1:A:92:ASN:ND2	1:A:103:HIS:CE1	2.77	0.51
1:B:71:ILE:O	1:B:79:ARG:HD2	2.11	0.51
1:B:138:LYS:HB3	1:B:144:ILE:HG12	1.92	0.51
1:B:338:ASP:O	1:B:363:LYS:HD2	2.11	0.51
1:A:319:PRO:HB2	1:A:353:CYS:SG	2.51	0.50
1:B:175:LYS:C	1:B:180:LYS:HD3	2.36	0.50
1:B:201:ARG:HH22	1:B:254:LEU:H	1.58	0.50
1:B:32:ARG:HG3	1:B:32:ARG:NH1	2.26	0.50
1:A:108:LEU:HD12	1:B:182:CYS:SG	2.52	0.50
1:B:43:ARG:HG3	1:B:44:SER:O	2.11	0.50
1:B:364:VAL:HG12	1:B:365:ASN:OD1	2.12	0.50
1:B:388:ILE:O	1:B:392:LEU:HD12	2.12	0.50
1:A:73:ARG:HH22	1:A:390:ARG:HH21	1.60	0.50
1:A:114:TYR:CD1	1:A:115:SER:N	2.80	0.50
1:B:52:GLY:HA2	1:B:243:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:PRO:HB2	1:B:353:CYS:SG	2.52	0.50
1:B:246:ARG:O	1:B:249:VAL:HG23	2.12	0.49
1:A:31:LYS:HB3	1:A:301:ARG:NH1	2.27	0.49
1:B:61:TYR:CD1	1:B:65:ASN:ND2	2.80	0.49
1:B:153:GLU:HG2	1:B:377:LEU:HB2	1.95	0.49
1:A:69:GLU:HB3	1:A:229:LEU:HD13	1.94	0.49
1:A:76:GLU:HA	1:A:79:ARG:NH2	2.27	0.49
1:B:212:TYR:CD1	1:B:249:VAL:HG21	2.47	0.49
1:A:319:PRO:HD3	1:A:403:CYS:HB3	1.94	0.49
1:B:139:ILE:HA	1:B:144:ILE:O	2.13	0.48
1:B:305:PHE:CD1	1:B:305:PHE:C	2.91	0.48
1:B:315:MET:HG3	1:B:404:ILE:O	2.13	0.48
1:B:61:TYR:CE1	1:B:65:ASN:ND2	2.81	0.48
1:A:216:TYR:CD2	1:A:247:PRO:HG2	2.48	0.48
1:A:393:LYS:O	1:A:396:GLN:HG3	2.13	0.48
1:B:63:LEU:HD23	1:B:106:ALA:CB	2.42	0.48
1:B:342:ILE:HD11	1:B:359:ILE:HD13	1.96	0.48
1:A:301:ARG:NH2	1:A:415:ILE:HD12	2.27	0.48
1:B:43:ARG:NH2	1:B:242:ASP:OD1	2.46	0.48
1:B:118:PHE:CD1	1:B:119:VAL:N	2.82	0.48
1:A:46:ILE:HG22	1:A:277:SER:HB3	1.95	0.48
1:A:317:VAL:HG12	1:A:317:VAL:O	2.14	0.48
1:B:307:THR:HA	1:B:409:GLY:O	2.12	0.48
1:B:43:ARG:HH21	1:B:228:ILE:HD11	1.78	0.48
1:A:315:MET:HE2	1:A:403:CYS:SG	2.53	0.47
1:A:42:ASN:OD1	1:A:73:ARG:NH1	2.48	0.47
1:A:58:ASN:HD22	1:A:59:THR:H	1.62	0.47
1:B:73:ARG:NH2	1:B:390:ARG:NH2	2.63	0.47
1:B:126:SER:O	1:B:130:THR:HG23	2.14	0.47
1:A:99:GLY:HA2	1:A:102:GLU:CD	2.39	0.47
1:A:102:GLU:HG2	1:A:103:HIS:H	1.80	0.47
1:A:416:LYS:HG3	1:A:417:GLU:OE1	2.15	0.47
1:B:94:LEU:HD11	1:B:377:LEU:HD12	1.97	0.47
1:B:99:GLY:HA2	1:B:102:GLU:OE2	2.15	0.47
1:B:186:MET:SD	1:B:315:MET:CE	3.03	0.47
1:B:203:ASP:HA	1:B:206:GLU:CD	2.39	0.47
1:B:232:LYS:HG3	1:B:238:ILE:CG1	2.45	0.47
1:A:117:PRO:CB	1:B:123:ARG:HH21	2.23	0.46
1:A:393:LYS:O	1:A:394:LYS:C	2.57	0.46
1:B:201:ARG:NH2	1:B:254:LEU:H	2.13	0.46
1:A:86:GLU:HG3	1:A:144:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:O	1:B:108:LEU:HG	2.16	0.46
1:B:224:PHE:HB3	1:B:228:ILE:CD1	2.45	0.46
1:B:244:GLY:H	1:B:245:PRO:CD	2.26	0.46
1:B:291:ALA:O	1:B:295:ASN:N	2.49	0.46
1:A:181:LYS:HA	1:A:184:ILE:HG12	1.97	0.46
1:A:190:ASN:ND2	1:A:346:PHE:CB	2.79	0.46
1:B:246:ARG:HH11	1:B:249:VAL:HG22	1.80	0.46
1:B:402:MET:O	1:B:402:MET:HG2	2.14	0.46
1:B:347:ALA:HB2	1:B:371:ILE:HD11	1.98	0.45
1:A:32:ARG:HB2	1:A:34:GLU:HG2	1.99	0.45
1:B:61:TYR:O	1:B:65:ASN:ND2	2.50	0.45
1:A:81:ASP:OD2	1:A:84:LEU:HD21	2.17	0.45
1:A:109:ALA:HB2	1:B:179:ALA:HB2	1.98	0.45
1:A:155:MET:HE1	1:A:375:HIS:O	2.16	0.45
1:A:157:ASN:H	1:A:157:ASN:HD22	1.64	0.45
1:B:304:ASP:CG	1:B:305:PHE:H	2.25	0.45
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.79	0.45
1:A:311:PRO:HB2	1:A:314:ILE:HG12	1.99	0.45
1:A:175:LYS:HG2	1:A:180:LYS:HZ2	1.81	0.45
1:B:177:ARG:HG2	1:B:178:GLU:N	2.31	0.45
1:A:181:LYS:HB3	1:A:312:PRO:HB2	1.98	0.45
1:A:280:VAL:CG1	1:A:281:ALA:N	2.80	0.45
1:B:42:ASN:HD22	1:B:229:LEU:CD1	2.29	0.45
1:B:57:VAL:HG13	1:B:61:TYR:HB3	1.99	0.45
1:B:301:ARG:HE	1:B:303:ILE:HD11	1.82	0.45
1:A:400:VAL:O	1:A:411:ALA:HA	2.16	0.44
1:B:46:ILE:HD11	1:B:383:ARG:HD2	1.98	0.44
1:A:385:VAL:O	1:A:388:ILE:HG22	2.17	0.44
1:B:404:ILE:HD11	1:B:410:ALA:HB2	1.99	0.44
1:A:63:LEU:O	1:A:67:LEU:HD22	2.18	0.44
1:A:174:GLN:OE1	1:A:175:LYS:N	2.51	0.44
1:A:315:MET:CE	1:A:403:CYS:SG	3.05	0.44
1:B:43:ARG:HA	1:B:281:ALA:HA	1.99	0.44
1:A:216:TYR:HD2	1:A:247:PRO:HG2	1.82	0.44
1:A:350:ALA:O	1:A:354:ILE:HG13	2.17	0.44
1:B:67:LEU:HD12	1:B:67:LEU:HA	1.81	0.44
1:A:224:PHE:CZ	1:A:367:ARG:HB3	2.52	0.44
1:B:123:ARG:O	1:B:124:GLN:HB2	2.17	0.44
1:B:288:ARG:HG3	1:B:288:ARG:NH1	2.33	0.44
1:A:33:PRO:HA	1:A:288:ARG:HB3	2.00	0.44
1:B:340:PHE:CD2	1:B:359:ILE:HG23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TYR:CE1	1:A:372:ALA:HA	2.53	0.44
1:B:100:ALA:HB2	1:B:120:ALA:CB	2.45	0.44
1:A:204:GLN:OE1	1:A:348:ALA:HB2	2.17	0.44
1:B:148:LEU:HD23	1:B:283:VAL:O	2.18	0.44
1:B:47:GLY:O	1:B:277:SER:HB3	2.18	0.44
1:B:364:VAL:O	1:B:365:ASN:C	2.61	0.44
1:A:66:PHE:CB	1:A:280:VAL:HG11	2.48	0.43
1:B:393:LYS:HB2	1:B:396:GLN:OE1	2.17	0.43
1:A:384:GLN:HE22	1:A:402:MET:HE3	1.83	0.43
1:B:178:GLU:O	1:B:181:LYS:HG2	2.18	0.43
1:B:250:THR:O	1:B:251:ALA:HB2	2.18	0.43
1:A:28:LEU:C	1:A:30:GLU:H	2.26	0.43
1:A:182:CYS:SG	1:A:406:THR:HG22	2.58	0.43
1:B:314:ILE:HG13	1:B:314:ILE:O	2.17	0.43
1:B:86:GLU:HB2	1:B:144:ILE:HG22	2.00	0.43
1:A:190:ASN:ND2	1:A:346:PHE:HB2	2.34	0.43
1:A:351:LEU:O	1:A:354:ILE:HB	2.19	0.43
1:B:89:ALA:HB2	1:B:134:ASP:OD2	2.19	0.43
1:B:405:GLY:C	1:B:407:GLY:H	2.26	0.43
1:A:77:PRO:O	1:A:80:ALA:HB3	2.19	0.43
1:A:402:MET:O	1:A:402:MET:HG2	2.18	0.43
1:A:201:ARG:HG2	1:A:205:ASP:OD2	2.19	0.43
1:B:78:LEU:O	1:B:81:ASP:N	2.51	0.43
1:B:183:LEU:H	1:B:406:THR:HG22	1.84	0.43
1:B:323:ILE:O	1:B:326:VAL:HG12	2.19	0.43
1:A:67:LEU:O	1:A:71:ILE:HG13	2.19	0.43
1:A:180:LYS:O	1:A:183:LEU:HB2	2.18	0.43
1:A:305:PHE:HE1	1:A:307:THR:OG1	2.02	0.43
1:B:28:LEU:O	1:B:28:LEU:HD23	2.19	0.43
1:B:122:ASN:OD1	1:B:122:ASN:C	2.62	0.43
1:A:29:LEU:HD13	1:A:415:ILE:HD13	2.00	0.42
1:A:81:ASP:C	1:A:83:ASN:N	2.77	0.42
1:B:78:LEU:O	1:B:80:ALA:N	2.52	0.42
1:A:33:PRO:HB2	1:A:289:SER:OG	2.20	0.42
1:A:121:LEU:HD12	1:A:121:LEU:N	2.34	0.42
1:A:190:ASN:ND2	1:A:348:ALA:HB3	2.32	0.42
1:B:155:MET:HB2	1:B:277:SER:O	2.18	0.42
1:A:78:LEU:O	1:A:82:LEU:N	2.53	0.42
1:A:315:MET:HG3	1:A:404:ILE:O	2.19	0.42
1:B:307:THR:HG22	1:B:308:VAL:N	2.35	0.42
1:A:244:GLY:N	1:A:245:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:O	1:B:161:ASN:ND2	2.52	0.42
1:A:156:THR:HG23	1:A:278:ASP:OD2	2.20	0.42
1:B:48:LYS:HB2	1:B:48:LYS:NZ	2.35	0.42
1:A:187:GLY:O	1:A:190:ASN:HB3	2.19	0.42
1:B:122:ASN:OD1	1:B:124:GLN:NE2	2.53	0.42
1:A:72:GLY:C	1:A:74:PHE:H	2.27	0.42
1:B:246:ARG:NH1	1:B:246:ARG:CG	2.81	0.42
1:A:43:ARG:HH21	1:A:228:ILE:HD11	1.85	0.42
1:A:303:ILE:HD13	1:A:303:ILE:HA	1.81	0.42
1:B:224:PHE:HB3	1:B:228:ILE:HD12	2.01	0.42
1:B:190:ASN:ND2	1:B:348:ALA:HB3	2.32	0.42
1:A:381:GLY:HA2	1:A:402:MET:HE1	2.02	0.41
1:B:42:ASN:ND2	1:B:73:ARG:HD2	2.34	0.41
1:B:303:ILE:HB	1:B:413:ILE:HG22	2.02	0.41
1:B:399:VAL:HG12	1:B:413:ILE:HG12	2.02	0.41
1:A:114:TYR:O	1:B:309:GLY:HA3	2.20	0.41
1:A:246:ARG:N	1:A:247:PRO:CD	2.83	0.41
1:B:285:LEU:N	1:B:285:LEU:HD22	2.35	0.41
1:A:275:GLN:NE2	1:A:372:ALA:O	2.53	0.41
1:A:399:VAL:HG12	1:A:413:ILE:HG12	2.02	0.41
1:A:56:ASP:O	1:A:57:VAL:HG23	2.21	0.41
1:A:290:VAL:O	1:A:293:GLN:HB2	2.20	0.41
1:B:71:ILE:HA	1:B:74:PHE:CD2	2.56	0.41
1:A:57:VAL:HG21	1:A:61:TYR:CD1	2.55	0.41
1:A:155:MET:CE	1:A:376:PRO:HA	2.51	0.41
1:B:42:ASN:HD22	1:B:229:LEU:CG	2.34	0.41
1:B:42:ASN:OD1	1:B:73:ARG:CZ	2.69	0.41
1:B:63:LEU:CD1	1:B:150:LEU:HD13	2.35	0.41
1:B:78:LEU:HD21	1:B:146:ILE:HD13	2.02	0.41
1:A:188:ILE:O	1:A:191:GLU:N	2.53	0.41
1:B:221:GLU:HB3	1:B:223:LEU:HG	2.03	0.41
1:A:158:ASN:C	1:A:160:LYS:H	2.28	0.41
1:A:323:ILE:HB	1:A:324:PRO:HD3	2.03	0.40
1:B:74:PHE:HA	1:B:75:PRO:HD3	1.96	0.40
1:A:116:THR:HG22	1:A:117:PRO:O	2.21	0.40
1:A:177:ARG:O	1:A:178:GLU:HB2	2.21	0.40
1:B:189:THR:HG22	1:B:313:GLU:O	2.21	0.40
1:B:333:GLN:O	1:B:334:VAL:C	2.64	0.40
1:A:86:GLU:O	1:A:87:GLU:CB	2.67	0.40
1:A:157:ASN:HD22	1:A:157:ASN:N	2.19	0.40
1:A:235:ASP:OD1	1:A:237:SER:OG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:PHE:CE1	1:B:284:LEU:HD22	2.56	0.40
1:B:133:ASN:HB2	1:B:305:PHE:CD2	2.56	0.40
1:B:48:LYS:O	1:B:52:GLY:N	2.55	0.40
1:B:86:GLU:HG3	1:B:144:ILE:CB	2.50	0.40
1:B:340:PHE:CD1	1:B:399:VAL:CG2	3.05	0.40
1:B:404:ILE:HB	1:B:408:MET:CB	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	335/390 (86%)	279 (83%)	46 (14%)	10 (3%)	3	12
1	B	338/390 (87%)	302 (89%)	24 (7%)	12 (4%)	2	10
All	All	673/780 (86%)	581 (86%)	70 (10%)	22 (3%)	3	11

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	B	177	ARG
1	B	178	GLU
1	B	182	CYS
1	B	251	ALA
1	B	377	LEU
1	A	55	LYS
1	A	178	GLU
1	A	405	GLY
1	B	52	GLY
1	B	405	GLY
1	A	50	PHE

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Mol	Chain	Res	Type
1	A	87	GLU
1	B	237	SER
1	A	29	LEU
1	A	124	GLN
1	A	236	GLY
1	B	87	GLU
1	B	156	THR
1	A	76	GLU
1	B	394	LYS
1	B	406	THR

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	273/311 (88%)	236 (86%)	37 (14%)	3	13
1	B	277/311 (89%)	239 (86%)	38 (14%)	3	13
All	All	550/622 (88%)	475 (86%)	75 (14%)	3	13

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	31	LYS
1	A	32	ARG
1	A	37	VAL
1	A	43	ARG
1	A	57	VAL
1	A	58	ASN
1	A	67	LEU
1	A	74	PHE
1	A	86	GLU
1	A	119	VAL
1	A	129	LEU
1	A	130	THR

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Mol	Chain	Res	Type
1	A	141	VAL
1	A	148	LEU
1	A	152	VAL
1	A	157	ASN
1	A	174	GLN
1	A	177	ARG
1	A	206	GLU
1	A	237	SER
1	A	277	SER
1	A	285	LEU
1	A	289	SER
1	A	299	LEU
1	A	310	VAL
1	A	313	GLU
1	A	315	MET
1	A	335	GLN
1	A	356	LYS
1	A	367	ARG
1	A	383	ARG
1	A	393	LYS
1	A	399	VAL
1	A	402	MET
1	A	406	THR
1	A	415	ILE
1	B	28	LEU
1	B	34	GLU
1	B	37	VAL
1	B	48	LYS
1	B	57	VAL
1	B	58	ASN
1	B	67	LEU
1	B	79	ARG
1	B	84	LEU
1	B	86	GLU
1	B	115	SER
1	B	129	LEU
1	B	135	ILE
1	B	141	VAL
1	B	148	LEU
1	B	152	VAL
1	B	159	TYR
1	B	161	ASN

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Mol	Chain	Res	Type
1	B	206	GLU
1	B	212	TYR
1	B	240	GLN
1	B	252	GLU
1	B	254	LEU
1	B	277	SER
1	B	285	LEU
1	B	302	TYR
1	B	310	VAL
1	B	313	GLU
1	B	315	MET
1	B	328	GLU
1	B	335	GLN
1	B	349	GLN
1	B	361	LEU
1	B	366	PRO
1	B	379	CYS
1	B	383	ARG
1	B	402	MET
1	B	417	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	65	ASN
1	A	83	ASN
1	A	103	HIS
1	A	124	GLN
1	A	157	ASN
1	A	190	ASN
1	A	192	ASN
1	A	295	ASN
1	A	335	GLN
1	A	365	ASN
1	A	384	GLN
1	B	42	ASN
1	B	58	ASN
1	B	65	ASN
1	B	158	ASN
1	B	190	ASN
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	213	GLN
1	B	220	ASN
1	B	275	GLN
1	B	292	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 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	343/390 (87%)	-0.44	1 (0%) 90 86	3, 25, 49, 70	0
1	B	348/390 (89%)	-0.58	1 (0%) 90 86	3, 20, 43, 65	0
All	All	691/780 (88%)	-0.51	2 (0%) 90 86	3, 23, 46, 70	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	PRO	2.1
1	B	183	LEU	2.1

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.