WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 07:15 AM EST

PDB ID	:	1PXT
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)

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

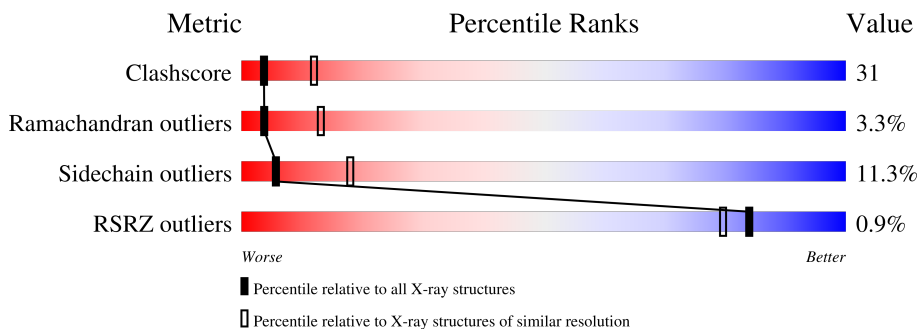|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Clashscore		31
Ramachandran outliers		3.3%
Sidechain outliers		11.3%
RSRZ outliers		0.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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.

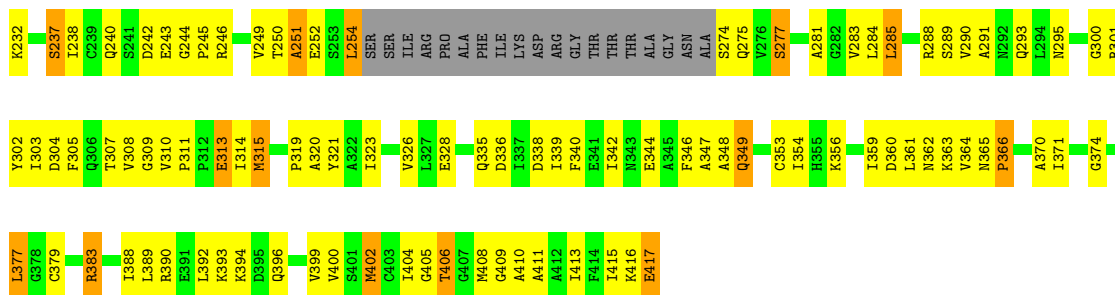| Mol	Chain	Length	Quality of chain
1	A	390	43% 39% 6% · 12%
1	B	390	37% 44% 8% 11%

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

Chain A:

● Molecule 1: PEROXISOMAL 3-KETOACYL-COA THIOLASE

Chain B:

K232 S237 I238 C239 Q240 S241 D242 E243 G244 P245 R246 V249 T250 A251 E252 S253 L254 SER SER ILE ARG PRO ALA PHE ILE LYS ASP ARG GLY THR THR THR ALA GLY ASN ALA S274 Q275 V276 S277 A281 G282 V283 L284 L285 R288 S289 V290 A291 N292 Q293 L294 N295 G300 R301

Y302 I303 D304 F305 Q306 T307 V308 G309 V310 P311 P312 E313 I314 M315 P319 A320 Y321 A322 I323 V326 L327 E328 Q335 D336 I337 D338 I339 F340 E341 I342 N343 E344 A345 F346 A347 A348 Q349 C353 I354 H355 K356 I359 D360 L361 N362 K363 V364 N365 P366 A370 I371 G374

L377 G378 C379 R383 I388 L389 R390 E391 L392 K393 K394 D395 Q396 V399 V400 S401 M402 C403 I404 G405 T406 G407 M408 G409 A410 A411 A412 I413 F414 I415 K416 E417

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 23.89 – 2.76	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 90.1 (23.89-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.35 , 104.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.62	0/2622	0.87	4/3543 (0.1%)
1	B	0.64	0/2651	0.90	2/3581 (0.1%)
All	All	0.63	0/5273	0.89	6/7124 (0.1%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	152	VAL	CB-CA-C	-5.65	100.67	111.40
1	B	121	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	285	LEU	CA-CB-CG	5.35	127.59	115.30
1	B	52	GLY	N-CA-C	5.33	126.41	113.10
1	A	119	VAL	CB-CA-C	-5.21	101.49	111.40
1	A	367	ARG	CG-CD-NE	5.10	122.51	111.80

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	157	0
1	B	2616	0	2655	183	0
All	All	5201	0	5283	327	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 31.

All (327) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ILE:HB	1:B:408:MET:HB2	1.69	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:A:126:SER:HA	1:A:402:MET:HE2	1.75	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:344:GLU:CD	1:A:369:GLY:HA3	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:126:SER:HA	1:B:402:MET:CE	2.37	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: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: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
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:186:MET:SD	1:B:315:MET:HE3	2.48	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: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:81:ASP:C	1:A:83:ASN:H	2.13	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASP:O	1:B:84:LEU:HB2	2.11	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: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:82:LEU:C	1:B:84:LEU:H	2.15	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
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:155:MET:HE2	1:A:377:LEU:H	1.77	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: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:118:PHE:CD1	1:B:118:PHE:C	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:104:ARG:O	1:B:104:ARG:HG3	2.16	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
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:175:LYS:C	1:B:180:LYS:HD3	2.36	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:157:ASN:H	1:A:157:ASN:HD22	1.64	0.45
1:A:280:VAL:CG1	1:A:281:ALA:N	2.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:305:PHE:CD1	1:B:305:PHE:C	2.91	0.44
1:B:47:GLY:O	1:B:277:SER:HB3	2.18	0.44
1:A:66:PHE:CB	1:A:280:VAL:HG11	2.48	0.43
1:A:381:GLY:HA2	1:A:402:MET:HE1	2.00	0.43
1:B:393:LYS:HB2	1:B:396:GLN:OE1	2.17	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: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: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:A:29:LEU:HD13	1:A:415:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:203:ASP:HA	1:B:206:GLU:CD	2.39	0.42
1:A:99:GLY:HA2	1:A:102:GLU:CD	2.39	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: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: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:393:LYS:O	1:A:394:LYS:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:304:ASP:CG	1:B:305:PHE:H	2.25	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
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 ⓘ

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	335/390 (86%)	279 (83%)	46 (14%)	10 (3%)	4	15
1	B	338/390 (87%)	302 (89%)	24 (7%)	12 (4%)	3	11
All	All	673/780 (86%)	581 (86%)	70 (10%)	22 (3%)	4	13

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	B	177	ARG
1	B	178	GLU

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Mol	Chain	Res	Type
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
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%)	248 (91%)	25 (9%)	9	27
1	B	277/311 (89%)	240 (87%)	37 (13%)	4	12
All	All	550/622 (88%)	488 (89%)	62 (11%)	6	18

All (62) 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	43	ARG

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Mol	Chain	Res	Type
1	A	58	ASN
1	A	67	LEU
1	A	74	PHE
1	A	119	VAL
1	A	129	LEU
1	A	141	VAL
1	A	148	LEU
1	A	177	ARG
1	A	206	GLU
1	A	220	ASN
1	A	277	SER
1	A	285	LEU
1	A	289	SER
1	A	310	VAL
1	A	315	MET
1	A	335	GLN
1	A	367	ARG
1	A	383	ARG
1	A	393	LYS
1	A	402	MET
1	A	406	THR
1	B	28	LEU
1	B	34	GLU
1	B	37	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	118	PHE
1	B	129	LEU
1	B	141	VAL
1	B	148	LEU
1	B	152	VAL
1	B	159	TYR
1	B	161	ASN
1	B	203	ASP
1	B	206	GLU
1	B	212	TYR
1	B	240	GLN
1	B	254	LEU

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Mol	Chain	Res	Type
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	336	ASP
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	65	ASN
1	A	103	HIS
1	A	157	ASN
1	A	158	ASN
1	A	190	ASN
1	A	295	ASN
1	A	335	GLN
1	A	384	GLN
1	B	42	ASN
1	B	58	ASN
1	B	65	ASN
1	B	83	ASN
1	B	158	ASN
1	B	190	ASN
1	B	192	ASN
1	B	213	GLN
1	B	275	GLN
1	B	292	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	343/390 (87%)	-0.45	4 (1%)	79	73	3, 25, 49, 70	0
1	B	348/390 (89%)	-0.55	2 (0%)	89	86	3, 20, 43, 65	0
All	All	691/780 (88%)	-0.50	6 (0%)	84	80	3, 23, 46, 70	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	LEU	2.7
1	A	247	PRO	2.4
1	A	331	GLY	2.3
1	A	28	LEU	2.3
1	B	176	ASN	2.1
1	A	177	ARG	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.