Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2024 – 12:13 am GMT

PDB ID	:	8OSY
Title	:	Trimeric catalytic domain of the E. coli Dihydrolipoamide Acetyltransferase (E2) of the pyruvate dehydrogenase complex
Authors	:	Meinhold, S.; Zdanowicz, R.; Glockshuber, R.
Deposited on	:	2023-04-20
Resolution	:	1.89 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:

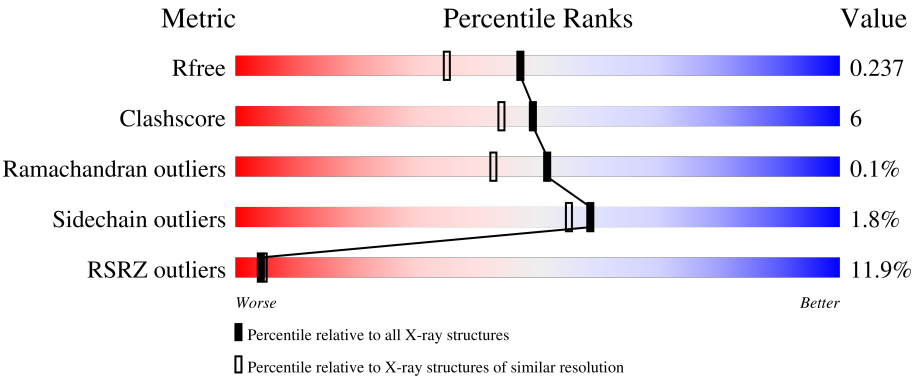
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	247	9% 88% 11%
1	B	247	2% 88% 11%
1	C	247	9% 92% 7%
1	D	247	28% 75% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8096 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 Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1901	1214	331	347	9			
1	B	245	Total	C	N	O	S	0	0	0
			1901	1214	331	347	9			
1	C	245	Total	C	N	O	S	0	1	0
			1910	1219	333	349	9			
1	D	245	Total	C	N	O	S	0	0	0
			1901	1214	331	347	9			

- Molecule 2 is water.

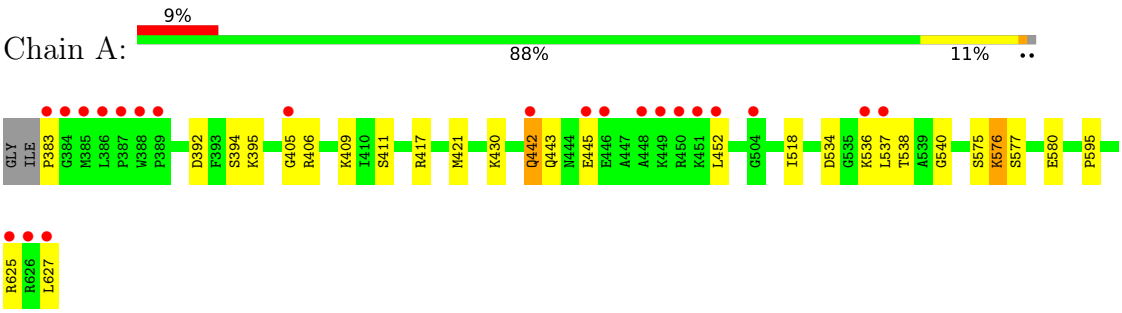
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	142	Total	O	0	0
			142	142		
2	B	180	Total	O	0	0
			180	180		
2	C	150	Total	O	0	0
			150	150		
2	D	11	Total	O	0	0
			11	11		

3 Residue-property plots (i)

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.

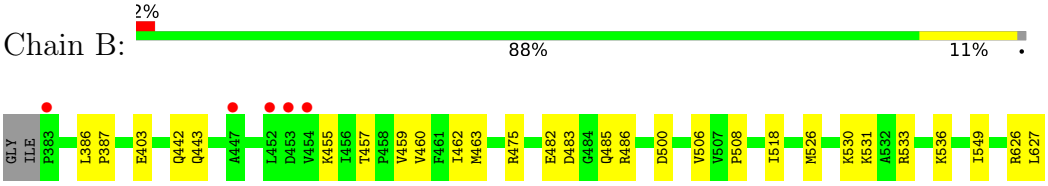
• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain A:



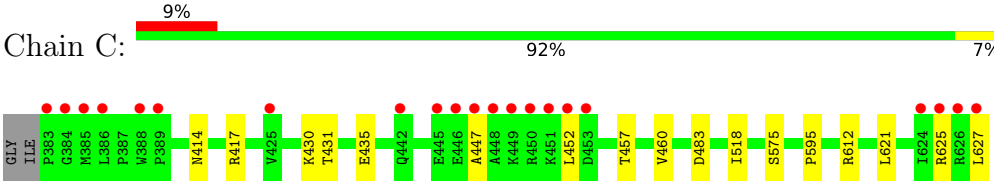
• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain B:



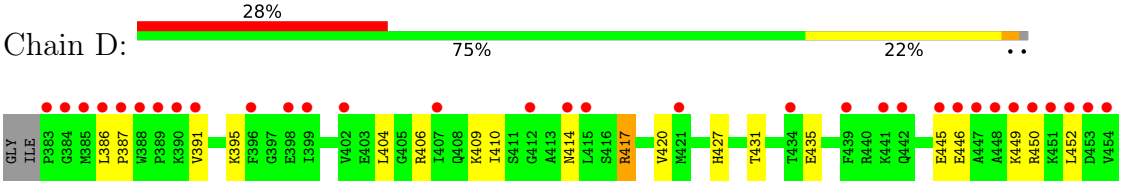
• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

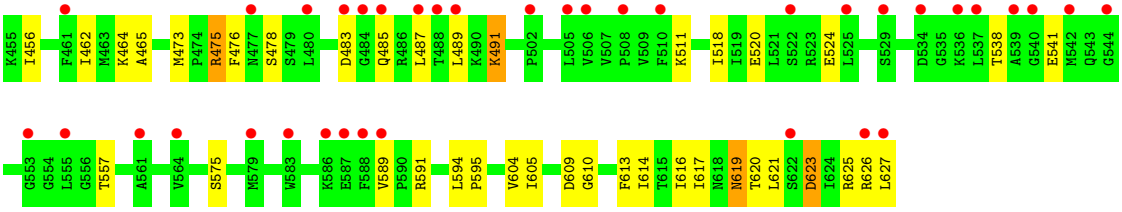
Chain C:



• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain D:




K455
I456
F461
I462
M463
K464
A465
M473
P474
R475
F476
N477
S478
S479
L480
D483
G484
Q485
R486
L487
T488
L489
K490
K491
P502
L505
V506
V507
P508
V509
F510
K511
I518
I519
E520
L521
S522
R523
E524
L525
S529
D534
G535
K536
L537
T538
A539
G540
E541
M542
Q543
G544
G553
G554
L555
G556
T557
A561
V564
S575
M579
W583
K586
E587
F588
V589
P590
R591
L594
P595
V604
I605
D609
G610
F613
I614
T615
I616
I617
M618
N619
T620
L621
S622
D623
I624
R625
R626
L627

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	148.15Å 148.15Å 119.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.96 – 1.89 44.96 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.96-1.89) 99.8 (44.96-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.244 0.199 , 0.237	Depositor DCC
R_{free} test set	3951 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8096	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.33	0/1936	0.57	0/2613
1	B	0.33	0/1936	0.56	0/2613
1	C	0.33	0/1945	0.57	0/2625
1	D	0.28	0/1936	0.54	0/2613
All	All	0.32	0/7753	0.56	0/10464

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1901	0	1967	21	0
1	B	1901	0	1967	19	0
1	C	1910	0	1974	13	0
1	D	1901	0	1967	43	0
2	A	142	0	0	0	0
2	B	180	0	0	2	0
2	C	150	0	0	1	0
2	D	11	0	0	0	0
All	All	8096	0	7875	91	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 6.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ASN:OD1	1:D:417:ARG:NH1	1.70	1.23
1:D:414:ASN:CG	1:D:417:ARG:HH12	1.40	1.22
1:D:414:ASN:HA	1:D:417:ARG:NH1	1.67	1.10
1:D:414:ASN:HA	1:D:417:ARG:HH11	1.16	1.10
1:D:414:ASN:CG	1:D:417:ARG:NH1	2.19	0.88
1:D:414:ASN:CA	1:D:417:ARG:NH1	2.42	0.82
1:B:518:ILE:H	1:B:627:LEU:HD23	1.48	0.79
1:B:526:MET:O	1:B:530:LYS:HD3	1.83	0.79
1:D:518:ILE:H	1:D:627:LEU:HD22	1.49	0.76
1:A:383:PRO:HD3	1:C:483:ASP:HA	1.67	0.75
1:B:386:LEU:HD12	1:B:387:PRO:HD2	1.72	0.71
1:D:478:SER:HB2	1:D:487:LEU:HD11	1.75	0.69
1:D:414:ASN:CB	1:D:417:ARG:NH1	2.59	0.66
1:A:430:LYS:HE2	1:A:580:GLU:OE2	1.96	0.64
1:A:576:LYS:HD3	1:A:577:SER:N	2.11	0.64
1:C:414:ASN:HD22	1:C:417:ARG:NH2	1.95	0.64
1:C:414:ASN:HD22	1:C:417:ARG:HH22	1.47	0.62
1:B:530:LYS:HD2	1:B:533:ARG:HH22	1.66	0.61
1:A:406:ARG:HB2	1:D:623:ASP:HB3	1.83	0.60
1:C:518:ILE:HB	1:C:627:LEU:HB3	1.84	0.59
1:D:478:SER:HB3	1:D:489:LEU:HD23	1.83	0.58
1:D:626:ARG:HB3	1:D:627:LEU:HD12	1.86	0.58
1:D:616:ILE:O	1:D:620:THR:HG22	2.04	0.58
1:D:475:ARG:O	1:D:478:SER:OG	2.19	0.57
1:D:404:LEU:O	1:D:409:LYS:NZ	2.35	0.55
1:A:442:GLN:NE2	1:A:443:GLN:OE1	2.35	0.55
1:D:476:PHE:CE1	1:D:605:ILE:HD12	2.42	0.54
1:A:625:ARG:HH11	1:A:625:ARG:HG3	1.73	0.54
1:D:610:GLY:O	1:D:614:ILE:HG22	2.08	0.54
1:B:486:ARG:NH2	2:B:701:HOH:O	2.23	0.53
1:A:392:ASP:OD1	1:A:394:SER:OG	2.25	0.53
1:B:457:THR:O	1:B:460:VAL:HG12	2.09	0.53
1:D:417:ARG:HA	1:D:420:VAL:HG22	1.92	0.52
1:C:447:ALA:HA	1:C:452:LEU:HD12	1.90	0.52
1:D:538:THR:OG1	1:D:541:GLU:HG3	2.09	0.52
1:A:538:THR:HG22	1:A:540:GLY:N	2.26	0.51
1:D:386:LEU:HD12	1:D:387:PRO:HD2	1.92	0.51
1:C:435:GLU:OE1	1:C:625:ARG:NH2	2.43	0.51
1:A:392:ASP:O	1:A:395:LYS:HG3	2.11	0.51
1:A:442:GLN:HA	1:A:445:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ARG:HG3	1:B:475:ARG:HH11	1.76	0.50
1:B:626:ARG:O	1:B:627:LEU:HB2	2.12	0.50
1:A:518:ILE:H	1:A:627:LEU:HD23	1.78	0.49
1:B:475:ARG:HG3	1:B:475:ARG:NH1	2.28	0.48
1:B:500:ASP:OD2	1:C:612:ARG:NH2	2.40	0.48
1:D:445:GLU:O	1:D:449:LYS:HG3	2.13	0.48
1:A:409:LYS:HD3	1:B:485:GLN:OE1	2.14	0.47
1:A:405:GLY:O	1:A:409:LYS:HG3	2.15	0.47
1:A:417:ARG:O	1:A:421:MET:HG3	2.15	0.46
1:D:604:VAL:HG12	1:D:605:ILE:HG12	1.98	0.46
1:D:386:LEU:HD12	1:D:386:LEU:HA	1.73	0.46
1:B:442:GLN:OE1	1:B:443:GLN:NE2	2.47	0.46
1:D:575:SER:HB2	1:D:595:PRO:HG2	1.97	0.46
1:D:491:LYS:N	1:D:491:LYS:HD2	2.31	0.46
1:A:575:SER:HB2	1:A:595:PRO:HG2	1.98	0.45
1:D:450:ARG:HB2	1:D:452:LEU:HG	1.97	0.45
1:D:395:LYS:HE2	1:D:395:LYS:HA	1.98	0.45
1:A:625:ARG:HG3	1:A:625:ARG:NH1	2.32	0.45
1:A:538:THR:HG22	1:A:540:GLY:H	1.82	0.45
1:D:456:ILE:H	1:D:456:ILE:HD12	1.82	0.45
1:D:619:ASN:HD22	1:D:619:ASN:N	2.14	0.45
1:D:520:GLU:O	1:D:524:GLU:HG3	2.17	0.44
1:C:575:SER:HB2	1:C:595:PRO:HG2	2.00	0.44
1:B:459:VAL:O	1:B:463:MET:HG3	2.18	0.43
1:C:460:VAL:HG23	1:C:518:ILE:HD12	1.99	0.43
1:D:464:LYS:HE3	1:D:464:LYS:HB3	1.65	0.43
1:D:465:ALA:HB2	1:D:621:LEU:HG	2.00	0.43
1:D:446:GLU:O	1:D:450:ARG:HG3	2.17	0.43
1:D:431:THR:HG23	1:D:594:LEU:HB3	2.00	0.43
1:D:589:VAL:HG23	1:D:591:ARG:HG2	2.01	0.43
1:B:462:ILE:HG22	1:B:549:ILE:HD13	2.01	0.43
1:A:534:ASP:HB3	1:A:536:LYS:HE3	2.00	0.43
1:B:506:VAL:HG23	1:B:508:PRO:HD3	2.01	0.42
1:B:483:ASP:O	1:B:485:GLN:HG2	2.20	0.41
1:C:414:ASN:ND2	1:C:417:ARG:HH22	2.16	0.41
1:C:457:THR:O	1:C:460:VAL:HG22	2.20	0.41
1:D:462:ILE:HG12	1:D:621:LEU:HD11	2.02	0.41
1:D:473:MET:HE1	1:D:609:ASP:HB3	2.01	0.41
1:D:613:PHE:CE2	1:D:617:ILE:HD11	2.54	0.41
1:A:537:LEU:HD12	1:A:537:LEU:HA	1.88	0.41
1:B:626:ARG:NH1	2:B:706:HOH:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:O	1:A:452:LEU:HD23	2.20	0.41
1:B:530:LYS:HD2	1:B:533:ARG:NH2	2.33	0.41
1:C:430:LYS:HE3	2:C:810:HOH:O	2.20	0.41
1:A:406:ARG:HH11	1:D:623:ASP:CG	2.24	0.41
1:C:431:THR:HG21	1:C:621:LEU:HD23	2.03	0.41
1:D:406:ARG:HA	1:D:409:LYS:HD3	2.01	0.41
1:D:435:GLU:OE1	1:D:591:ARG:NH2	2.54	0.41
1:B:531:LYS:HG2	1:B:536:LYS:HB2	2.03	0.40
1:D:406:ARG:O	1:D:410:ILE:HD12	2.21	0.40
1:D:483:ASP:CG	1:D:485:GLN:HG2	2.42	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	243/247 (98%)	235 (97%)	8 (3%)	0	100	100
1	B	243/247 (98%)	239 (98%)	4 (2%)	0	100	100
1	C	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
1	D	243/247 (98%)	234 (96%)	8 (3%)	1 (0%)	34	24
All	All	973/988 (98%)	947 (97%)	25 (3%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	557	THR

5.3.2 Protein sidechains (i)

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	209/210 (100%)	206 (99%)	3 (1%)	67 65
1	B	209/210 (100%)	206 (99%)	3 (1%)	67 65
1	C	210/210 (100%)	210 (100%)	0	100 100
1	D	209/210 (100%)	200 (96%)	9 (4%)	29 19
All	All	837/840 (100%)	822 (98%)	15 (2%)	59 55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	SER
1	A	442	GLN
1	A	576	LYS
1	B	403	GLU
1	B	455	LYS
1	B	482	GLU
1	D	391	VAL
1	D	417	ARG
1	D	427	HIS
1	D	475	ARG
1	D	491	LYS
1	D	511	LYS
1	D	619	ASN
1	D	623	ASP
1	D	625	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	414	ASN
1	D	602	HIS
1	D	619	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, 95^{th} 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	245/247 (99%)	0.53	22 (8%) 9 10	27, 46, 80, 94	0
1	B	245/247 (99%)	0.24	5 (2%) 65 68	26, 45, 73, 102	0
1	C	245/247 (99%)	0.44	21 (8%) 10 12	27, 47, 91, 141	0
1	D	245/247 (99%)	1.60	69 (28%) 0 0	55, 87, 118, 157	0
All	All	980/988 (99%)	0.70	117 (11%) 4 5	26, 53, 106, 157	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	386	LEU	8.2
1	A	626	ARG	8.0
1	D	484	GLY	7.6
1	C	626	ARG	7.2
1	C	447	ALA	6.7
1	D	589	VAL	6.7
1	D	389	PRO	6.6
1	D	402	VAL	6.5
1	B	383	PRO	6.5
1	D	506	VAL	6.1
1	C	448	ALA	6.0
1	C	450	ARG	5.5
1	D	489	LEU	5.4
1	C	386	LEU	5.0
1	A	385	MET	4.9
1	D	540	GLY	4.9
1	D	627	LEU	4.8
1	D	488	THR	4.8
1	D	391	VAL	4.7
1	C	624	ILE	4.6
1	A	627	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	383	PRO	4.3
1	D	448	ALA	4.3
1	A	625	ARG	4.2
1	C	384	GLY	4.2
1	A	384	GLY	4.2
1	D	412	GLY	4.2
1	D	383	PRO	4.1
1	D	388	TRP	4.1
1	A	388	TRP	4.0
1	A	387	PRO	3.8
1	C	451	LYS	3.8
1	D	415	LEU	3.7
1	A	449	LYS	3.7
1	B	452	LEU	3.7
1	D	502	PRO	3.7
1	D	525	LEU	3.7
1	D	442	GLN	3.7
1	C	442	GLN	3.6
1	C	383	PRO	3.6
1	A	405	GLY	3.6
1	D	439	PHE	3.6
1	D	553	GLY	3.6
1	C	627	LEU	3.5
1	A	450	ARG	3.5
1	D	390	LYS	3.5
1	D	537	LEU	3.5
1	A	451	LYS	3.4
1	D	407	ILE	3.4
1	D	387	PRO	3.4
1	C	452	LEU	3.4
1	D	487	LEU	3.3
1	C	385	MET	3.3
1	C	449	LYS	3.3
1	C	446	GLU	3.2
1	D	452	LEU	3.2
1	D	414	ASN	3.2
1	D	544	GLY	3.2
1	D	564	VAL	3.2
1	C	453	ASP	3.1
1	D	385	MET	3.1
1	D	450	ARG	3.1
1	D	583	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	539	ALA	3.1
1	A	386	LEU	3.0
1	D	588	PHE	3.0
1	D	449	LYS	3.0
1	D	399	ILE	2.9
1	B	454	VAL	2.8
1	A	442	GLN	2.8
1	D	510	PHE	2.8
1	D	485	GLN	2.8
1	A	452	LEU	2.8
1	D	626	ARG	2.8
1	A	448	ALA	2.7
1	D	579	MET	2.7
1	D	483	ASP	2.7
1	D	396	PHE	2.6
1	D	454	VAL	2.6
1	D	508	PRO	2.6
1	D	529	SER	2.6
1	D	446	GLU	2.6
1	D	451	LYS	2.6
1	A	389	PRO	2.6
1	D	398	GLU	2.5
1	D	505	LEU	2.5
1	A	445	GLU	2.5
1	B	453	ASP	2.5
1	B	447	ALA	2.4
1	D	480	LEU	2.4
1	D	536	LYS	2.4
1	D	622	SER	2.4
1	D	555	LEU	2.4
1	D	384	GLY	2.4
1	D	587	GLU	2.4
1	C	445	GLU	2.4
1	C	388	TRP	2.3
1	A	536	LYS	2.3
1	D	447	ALA	2.3
1	D	461	PHE	2.3
1	D	586	LYS	2.3
1	A	446	GLU	2.3
1	D	542	MET	2.2
1	D	453	ASP	2.2
1	D	441	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	421	MET	2.2
1	D	477	ASN	2.2
1	C	425	VAL	2.1
1	D	534	ASP	2.1
1	D	434	THR	2.1
1	C	625	ARG	2.1
1	D	561	ALA	2.1
1	A	537	LEU	2.1
1	A	504	GLY	2.1
1	D	445	GLU	2.0
1	C	389	PRO	2.0
1	D	522	SER	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 monosaccharides 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.